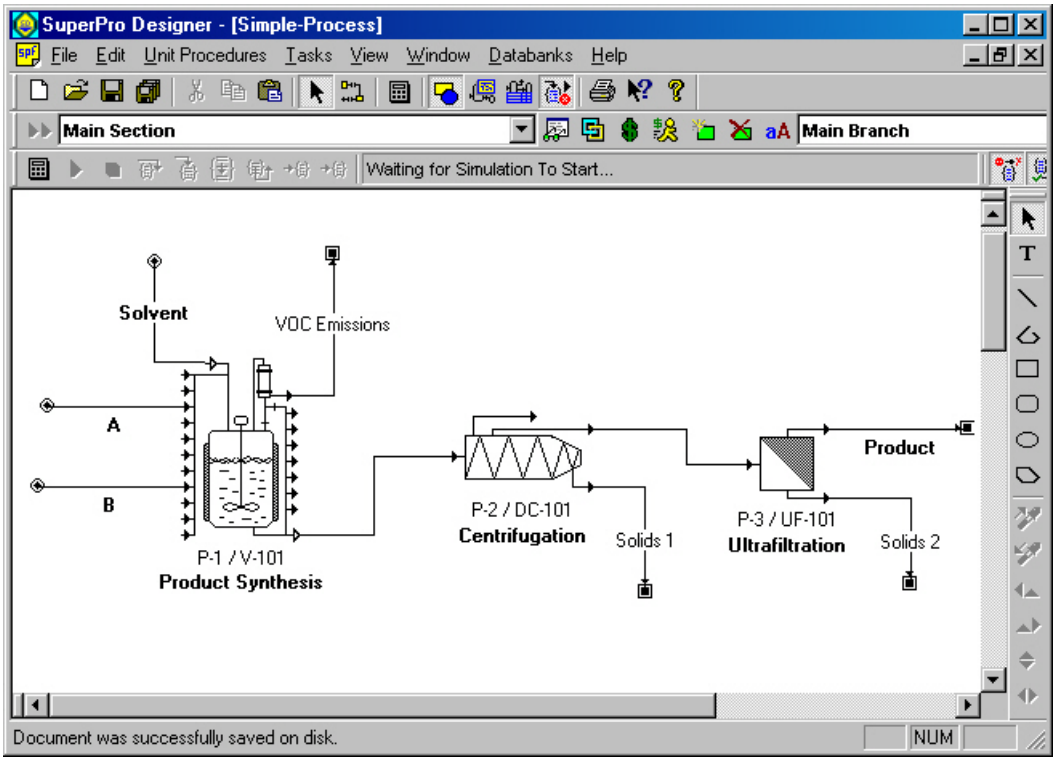
SuperPro Designer®

User Guide



A Comprehensive Simulation Tool for the Design, Retrofit & Evaluation of Specialty Chemical, Biochemical, Pharmaceutical, Consumer Product, Food, Agricultural, Mineral Processing, Packaging

AND

Water Purification, Wastewater Treatment and Air Pollution Control Processes.

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1

GETTING STARTED

Welcome to Intelligen's family of simulation software. Whether you acquired SuperPro Designer or EnviroPro Designer you have now joined a large group of professionals (engineers and scientists) from the industry and the academia who have used this software for well over twenty five years in order to meet their every day challenges in process simulation and related activities such as: process economics and profitability assessment, retrofit and debottlenecking studies, environmental impact assessment, emission reporting just to name few such simulation-related activities that are currently being done by the users of this software. Here's a partial list of companies that are currently relying on our software to meet their simulation challenges: Amgen, Abbott Laboratories, ADM, Baxter, Bayer Technology Services (Europe and USA), Biogen Idec, Bio-Rad Laboratories, Bio-Springer (France), Bristol-Myers Squibb, Cangene (Canada), CDI, Centocor, CH2M Hill, Chugai Pharmaceuticals (Japan), CJ Corporation (Korea), Colgate Palmolive, Crucell (Holland), CRB Engineers, Dow Chemical, DuPont, Eli Lilly, Fluor, FMC BioPolymer, Foster Wheeler (UK), GE Healthcare, Genencor, Genentech, Genmab (Denmark and USA), GlaxoSmithKline, Hitachi Plant (Japan), Hoffmann-La Roche (multiple sites), Human Genome Sciences, Jacobs Engineering, Janssen (Belgium), Laporte Consultants (Canada), Lonza (multiple sites), Medarex, MedImmune, Merck, Merck Serono (Switzerland), Monsanto, NNE Pharmaplan (Europe), Novartis, Petrobras (Brazil), Pfizer, Procter & Gamble, Regeneron, Roquette (France), SAIC-Frederick, Sandia National Laboratories, Sanofi-Pasteur (Europe, Canada, and USA), Talecris Biotherapeutics, U.S. DOA, DOD, DOE, Wyeth Pharmaceuticals. There are also over 300 universities worldwide that are using this software for as part of their course curriculum (as a teaching aid) or for applied research in the U.S. and abroad. For a more up-to-date list of industrial and academic users please visit our web site (www.intelligen.com)..

If you have purchased a copy of EnviroPro Designer please note that this manual was written with a SuperPro Designer user in mind. You probably noticed that the cover page mentions the name of SuperPro Designer right away instead of EnviroPro Designer. Please note that the two products share an identical interface and make use of the same exact tools (options) to tackle simulation and process evaluation issues. The only difference between the two tools is simply the number of modeling modules available (options under the Unit Procedures menu). EnviroPro Designer includes only a subset of the options that are available for SuperPro Designer users. The subset of options included in EnviroPro Designer are those modules most commonly needed to simulate processes in the water purification, wastewater treatment and air pollution control areas.

The SuperPro/EnviroPro Designer software is today's best option for any chemical, biochemical or environmental engineer and scientist in R&D, process engineering or manufacturing. Whether you are a member of a biochemical, pharmaceutical, specialty chemical, food company or whether you are employed by an environmental consulting firm or a water purification/treatment plant, you can benefit from making this product part of your

every day computing options. Its use will enhance the productivity and communication efficacy of all members in your group as well between your group and other parts of your organization.

SuperPro and EnviroPro Designer software manage a unique balance between flexibility, ease of use and computational power. They can be readily used by a computer novice who is not very familiar with simulation and economic evaluation. At the same time, in the hands of a simulation veteran, they can be used to model complex process situations under continuous or batch mode or both (mixed mode processes). Both programs use the same user-friendly interface thereby making it easy to migrate from one product to another as your needs may change in the future. And in case you stumble across a question, help is just one keystroke away. Hitting **F1** will present a help screen that is closely related to the chore you are currently executing. Besides offering information on your current task, the help screen will also provide you with a gateway into other (related) topics, all presented in an HTML based format that should be already familiar to all Windows users. The help system also allows you to search for topics related to keywords, jump from one help topic to another, and it is designed to help you 'learn-as-you-go'.

While we have made every effort to make the learning curve of our software as smooth and short as possible, at the same time, we have loaded it with several features that will satisfy even the simulation veteran when it comes to carry out any of the following tasks a part of a preliminary design and evaluation of process alternatives:

- Material and Energy Balances of Integrated Processes
- Equipment Sizing
- Scheduling and Cycle Time Analysis of Batch Processes
- Cost Analysis and Economic Evaluation
- Throughput Analysis and Debottlenecking
- Environmental Impact Assessment

All of the simulation results can also be viewed in the form of either self-contained reports (in PDF, MS-Word, HTML and many other formats) or they can be included as part of your own reports put together in Excel. Using the latest OLE technology, you can also copy all or parts of your flowsheet and/or any chart or other graph generated by the application and simply paste it in your favorite Windows application used to put together your report or presentation.

1.1 ABOUT THIS MANUAL

Most users do not like reading manuals cover-to-cover. We understand that, and therefore this manual was put together with that understanding in mind. However, as much as we have tried to make the use of the software as easy and intuitive as possible, we believe that any user can benefit from reading this manual. If you don't have time to read the entire manual, we strongly urge all users to (at least) skim through the contents of this manual in order to get an idea about some of the features of the software. As a minimum, please read through the first two chapters and use the rest of the material just for reference. Please note that the entire contents of this manual, plus additional information regarding modeling details of all the operation and equipment types supported by the software and more in-depth coverage of all the interfaces

(dialogs, charts, etc.) used by the software to interact with the user, are included in a PDF edition of the manual that is installed on your PC (assuming you included the Help/Documentation component during installation). This e-book version of the manual is copied along with the program files under the user-selected installation directory. The file's name is "EBook.pdf". A short-cut labeled accordingly has been installed under the "SuperPro Designer" program group (under your "Start" button of your desktop) and it can be viewed directly on your PC but it requires Adobe®'s Acrobat Reader® (v6 or later) to be present. If you don't have Adode®'s Acrobat Reader®, please visit http://get.adobe.com/reader/ and download and install the latest version (free of charge).

In this chapter, you will find some general and useful information regarding installation of the software on your PC, see 1.3 Installation. Also, if you have purchased an annual license of the software and you decide to extend your license for another term, you will find detailed information on how to execute this procedure, see 1.5 License Renewal. Chapter 2 includes a simple, step-by-step approach to what it takes to develop a process simulation using this program. The end goal is to represent a very simple process as a vehicle in demonstrating the principles and the most crucial elements of the user interface.

Please note that not all features of the software will be mentioned in the Tutorials included in Chapter 2 of this manual. Users are strongly encouraged to experiment and explore for more options available by reading the rest of the contents of this manual (or its E-Book equivalent), or browsing through the on-line help system that can be the perfect way to find out what a given menu option or button or dialog is supposed to do. Another option to become more familiar with all the options available in SuperPro Designer and climb the learning curve in a fast pace is to participate in one of our regularly scheduled training sessions taking place all over the world. For details on upcoming dates and locations of Intelligen's training please visit our web site (www.intelligen.com/traning.html). Finally, it is also possible to contact Intelligen, Inc. and arrange for an on-site training. This option is most suited for clients who have highly specialized simulation needs, as such on-site training will focus on your own organization's simulation needs.

In addition, three more examples are described in greater detailed. The first, which deals with the production of ß-galactosidase (or b-gal) is recommended for users in the biochemical and related industries. The second, which deals with a synthetic pharmaceutical process, is recommended for users in the pharmaceutical, agrochemical, and specialty chemical industries. The third, which analyzes an industrial wastewater treatment plant, is recommended for users in the environmental field of applications. Regardless of which example you chose, you will be presented with a comprehensive tour of all the basic features of the application and will be given all the pointers that you need in order to start your own simulations.

1.2 HARDWARE & SOFTWARE REQUIREMENTS

SuperPro Designer will run on any modern PC running Windows Vista, Win7, Win8 or Win8.1 (32- or 64-bit). The application itself is (natively) a 32-bit application and if installed on a 64-

bit Windows, it will run under the 32-bit compatibility mode (and thus will be installed under the "Program Files (x86)" system area.

Hard Disk Space	Depending on your choices during installation, the programs will occupy anywhere from 350 MB (for minimum installation) to 550 MB of space on your hard disk. The size depends on whether you chose to install all the example files and all files required for the on-line (context-sensitive) help and documentation support.
Processor /RAM	No special requirements needed over the minimum dictated by your operating system.
Mouse	The presence of a mouse or a similar pointing device supported by your Windows operating system is required.
Video Adapter & Monitor	No special requirements other than a minimum resolution of 1024 x 768 or better. A screen of 17" or better is strongly recommended for most comfortable use.
Printer	Any printer or plotter supported by your Windows environment.If you don't use a plotter and for best results a laser postscript printer with at least 4MB of memory is recommended.

1.3 INSTALLATION

Most versions of SuperPro Designer require the use of a hardware security key. Even though you will need to plug the key into a USB port on your PC before you can successfully boot up and continue to use the application, you do not need to plug in your sentinel key before you start the installation process! In fact, in order to facilitate the successful installation of the proper communication software required to communicate between our application and the sentinel key, you should not plug in the key until after the conclusion of the installation. The presence of the key is not needed in order for the installation to conclude successfully.

It is required that the application is installed by either a System Administrator or a user with System Administrator privileges. Please contact your IT professional to inquire if your user profile has such privileges. Also, please read through the relevant topics included in the 'ReadMe' file (located on the top-level of the installation CD) for more details regarding installation, installation requirements, and troubleshooting problems during installation.

As soon as you insert the installation CD into your drive, the setup program will start automatically. If the installation program doesn't start automatically (an option on your operating system may prevent this from happening) please right-click on your CD drive's image and start the installation program:
|'SuperPro Designer v<MajorVerNo>b<SBN>.exe' (e.g. "SuperPro Designer.v9.b04.exe"), on the CD manually.
<MajorVerNo> will be the major version number of the release you are installing (e.g. "9", "9.5" or "10").
<SBN> is the special build number of the release you are installing (e.g. "02", "05", "12", etc.)
For more details on the release number scheme for SuperPro Designer please consult the "ReadMe" file.

The installation program will accomplish the following tasks:

1. It will personalize your copy of the application for your organization and yourself.
2. It will copy all necessary files onto your hard disk at a directory of your choice.
3. It will make the necessary updates of your computer's registry.
4. It will create a program group and include in it entries to run the application, its help system, the license renewal utility or the PDF manual.

During installation you will be asked to provide the following information:

(a) Your name and the name of your organization.

(b) A folder where the application will be installed.

(c) Another folder where the application's database files will be installed.

(d) Which program configuration you want to install: Typical, Minimum or Custom. For most users the default ('Typical') is recommended. Depending on your choice, different sets of files will be copied. Custom installation will let you pick and choose what components you need copied on your disk. Minimum installation will only copy the files that are absolutely necessary for your program to run. It will not copy the help files and the example files. If your hard disk space allows, it is highly recommended that you install the help files as well as the example files. The examples contain several process files completed with the program, along with pertinent information for each case (in the form of a 'ReadMe' file). If you decide not to include the examples during the first installation, you can always run the setup program later and copy them to your hard disk at that time. To avoid re-installing the entire program, the second time, select "Custom" from the installation options, and pick only the "Example" component.

The installation process will overwrite any files with the same name that may reside in the specified installation folder. If have been using the application for a while and are now upgrading to a newer version, it is highly recommended that you either make backup copies of your current user database file or specify a new location.

It is recommended that you review the 'ReadMe' file either at the conclusion of program installation or at some other point before you start using your program for the first time. The 'ReadMe' file contains most important, up-to-date information about the release you have just installed, including all the latest features that have been added and/or issues that may have been addressed with that release.

1.4 TECHNICAL SUPPORT

Technical support is available for registered users with valid maintenance contracts. For users who purchase perpetual licenses, you must make sure you keep your maintenance contract active. This will entitle you for unlimited technical support. Also, should you run into an unexpected program behavior, Intelligen, Inc. will make every effort to resolve problem and issue a fix in short time. It is very important that you complete the registration sheet (green form) that was sent to you upon receipt of your original license or license renewal

confirmation. After you fill up (or inspect and correct) the registration form please use the pre-stamped (for US destinations only) envelope and mail it to:

Intelligen, Inc.

2326 Morse Ave.

Scotch Plains, NJ 07076, USA

If you have a valid maintenance contract and need to contact us for a technical support issue, here are your choices:

E-Mail (preferred)	TechSupport@intelligen.com
Phone (USA)	(908) 654-0088, 9am-5pm EST (262) 483-8846, 9am-5pm CT
Phone (Europe)	(+30) (2310) 472-670, 9am-5pm in Europe (Greece).

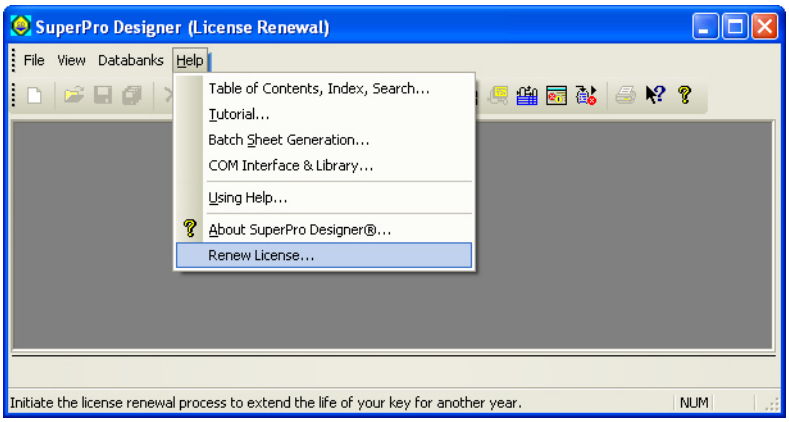
1.5 LICENSE RENEWAL

If you are licensing this program for a limited time (typically a year) you will find out that after the license expires, the program will give you few warnings and eventually will not start unless you renew your license. The license renewal process is very simple and, in most cases, it can be done from your own office. Before you start the license renewal procedure, you must purchase an extension to your license and in return you will be given a password that is to be used during the renewal process. Once you know your password, you are ready to start. Note that the password is only good for extending the license agreement for one term. The next time you need to extend your license for another term, you have to repeat the process and acquire another password.

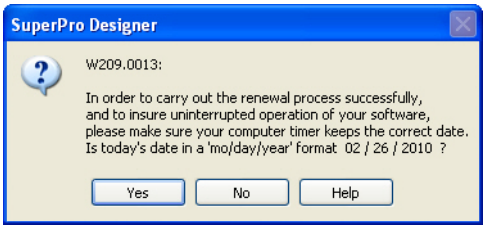
▶ To renew your license for another term...

1. Select 'Sentinel Key Renewal' from the 'Program Files' group where you normally start SuperPro Designer. Alternatively, you can double-click on the 'SPDLicenseRenewal.exe' executable located in the installation folder of SuperPro Designer.
2. Next, SuperPro Designer will appear in 'License Renewal' mode (see below). From the **Help** menu, please select **Renew License**
.

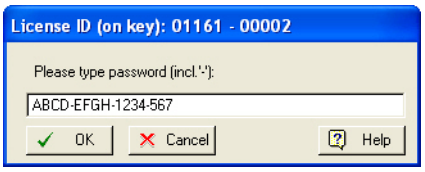
Before you initiate the license renewal process, please make sure that the time and date on your PC are accurate. If you attempt to execute the renewal process with a date that is not accurate, it is possible that the procedure will fail (either during the renewal process itself or soon after you restart SuperPro Designer) leading to a possible lock-out of the key. Once a key is locked out, then it is no longer usable. It must be returned to Intelligen, Inc. and a new key programmed correctly for your new expiration date will be issued and sent to you.


SuperPro Designer (License Renewal)
File View Databanks Help
Table of Contents, Index, Search...
Tutorial...
Batch Sheet Generation...
COM Interface & Library...
Using Help...
About SuperPro Designer®...
Renew License...
Initiate the license renewal process to extend the life of your key for another year.
NUM

and after you confirm that the reported time and date is correct, the password entry dialog (see step 3) will appear.

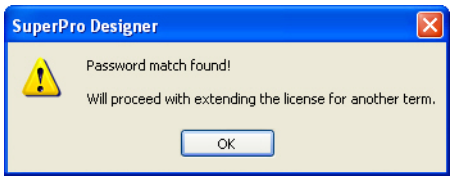

SuperPro Designer
W209.0013:
In order to carry out the renewal process successfully,
and to insure uninterrupted operation of your software,
please make sure your computer timer keeps the correct date.
Is today's date in a 'mo/day/year' format 02 / 26 / 2010 ?
Yes
No
Help

3. When the password entry dialog appears, please type in the password that was provided to you from Intelligen for this renewal process.

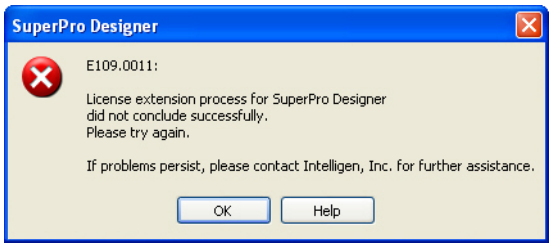


Please note that each password provided is only valid for one time. Also, the password is likely to be a combination of numbers, letters (in upper or lower case) and hyphens (‘-’).

4. If the password string that was typed matches with the information imprinted on the sentinel key, then the following message will appear:

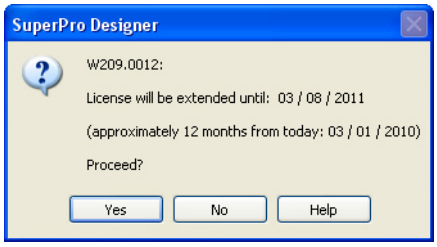


If for some reason, a match was not found then you will see the following notification:



If you are certain that you provided the correct password yet the renewal process cannot proceed beyond this point, please contact Intelligen, to resolve the issue. If we are unable to resolve the issue, a new key will be shipped to you and you will be asked to send your old key back.

5. The next dialog will show you the date that will be used as the next expiration date imprint on the key. If you agree, simply click **OK**. If you think that there has been an error in the calculation of the next expiration date, please contact Intelligen.If you confirm the date



then after clicking **OK**, the license renewal process concludes announcing success!

SuperPro Designer
License renewal finished successfully.
Please shut down SuperPro Designer and start again as usual.
OK

If you received the password electronically (via e-mail) it is recommended that you copy-and-paste it from the original notification that was sent to you from Intelligen, Inc.. This way, you will minimize the possibility of typographical errors which will lead to an unsuccessful completion of the renewal process.

NOTES

1. The first time you attempt to start your program after your license agreement has expired and you haven't renewed your license yet, a license violation will be detected and you will be prompted to proceed with acquiring a password to start the license renewal process. From that point on, you can only start the program again a few times before it locks itself. Once the program locks itself, the only way to get it unlocked is to contact Intelligen, Inc. and acquire a password in order to start the license renewal process described above.
2. You can only apply the above procedure on the same sentinel key for only a fixed number of times (currently it is 6 times). After that, you will have to send your old hardware key to Intelligen, Inc. in exchange for a new key that can be used for six more terms.

Although it is a rare case, it may be that your hardware key becomes defective and does not respond to the above renewal procedure. If that case presents itself, then simply mail your old key to Intelligen, Inc. and a new key will be sent out to you.

2

TUTORIAL

In this chapter, we will guide you through the steps of creating a process model in SuperPro Designer. We will first describe how to create a simple example process model. This example will illustrate the key initialization steps involved with the creation of any type of process. Regardless of which industry you are in, you should read through this example to become familiar with the basic steps of modeling processes using SuperPro Designer.

In addition to this simple example, three other process model examples will be described in this chapter. These examples, listed below, are more complex than the first one and they are better representations of what a "real" process modeled with SuperPro Designer would look like:

- *Synthetic Pharmaceuticals*. This example deals with a synthetic pharmaceutical process. It is recommended for users in the pharmaceutical and specialty chemical industries.
- *Biotech Processing*. This example deals with the production of β-galactosidase and it is recommended for users in the bioprocessing industries.
- *Wastewater Treatment*. The third additional example deals with an industrial wastewater treatment plant and it is recommended for users that target water purification and wastewater treatment applications.

The table below provides a brief description of all the examples that are shipped with SuperPro Designer and/or EnviroPro Designer (including those described in this chapter):

Folder Name	Available In	Description
AirContr	SuperPro /EnviroPro Designer	This example analyzes a three-step process for removing dust particles and acetone (a VOC molecule) from an air stream. It is recommended for users with interests in *air pollution control processes*.
AlgalOil	SuperPro Designer	This example provides a basic representation of an algae production and purification process that generates a lipid which could subsequently be converted into bio-diesel or jet fuel. It is recommended for users with interests in *biofuel processes*.
Bgal	SuperPro /EnviroPro Designer	This example deals with the production of β-galactosidase. It is recommended for users in the *bioprocessing industries*.

Folder Name	Available In	Description
BioDiesl	SuperPro /EnviroPro Designer	This example deals with the production of biodiesel from soybean oil and it is based on a process model developed by scientists at a research center of USDA. It is recommended for users who are interested in *biofuel processes*.
Brewery	SuperPro Designer	This example simulates the operation of an industrial beer production and packaging facility. It is recommended for users in the *brewing and beverage industries.*
Cheese	SuperPro Designer	This example analyzes a highly integrated dairy plant that produces cheese, butter, WPC, and ethanol. It is recommended for users with interests in *food processing*.
CitricAcid	SuperPro Designer	This example analyzes the production of citric acid via fermentation. It is recommended for users with interests in *commodity biochemicals*.
COM	SuperPro /EnviroPro Designer	This directory includes several examples of the COM interface capabilities of SuperPro Designer and EnviroPro Designer; for more details, see COM Library.
Ethanol	SuperPro Designer	This example deals with the production of ethanol from corn stover. It can be readily modified to represent conversion of other types of ligno-cellulosic biomass into ethanol. It is recommended for people that are interested in production of *biofuels* from renewable resources that do not compete with food supplies.
GE	SuperPro /EnviroPro Designer	This example analyzes an effort to minimize generation of hazardous sludge and wastewater at a manufacturing facility of General Electric. It is recommended for users with interests in *waste minimization*, *water recycling*, and *pollution control*.
Incinrtn	SuperPro /EnviroPro Designer	This example describes a simple process (a single unit) for analyzing the combustion of sludge in an incinerator. It is recommended for users with interests in *incineration* and *pollution control*.
IndWater	SuperPro /EnviroPro Designer	This example deals with an industrial wastewater treatment plant. It is recommended for users that target *water purification* and *wastewater treatment* applications.
Insulin	SuperPro Designer	This example analyzes the production of biosynthetic human insulin (a variation of Eli Lilly's process for Humulin). It is recommended for users with interests in *bioprocessing* and *biopharmaceuticals*.

Folder Name	Available In	Description
Lysine	SuperPro Designer	This example models a plant which produces 30,000 metric tons of the amino acid lysine annually. Lysine is produced industrially by microbial fermentation. This example is recommended for users with interest in *commodity biochemicals*.
MAB	SuperPro Designer	This example analyzes the production of a therapeutic monoclonal antibody using animal cell culture. It is recommended for users with interests in *animal cell culture* and *high value biopharmaceuticals*.
Misc	SuperPro /EnviroPro Designer	This directory includes a number of small examples that demonstrate key features of SuperPro Designer.
MunWater	SuperPro /EnviroPro Designer	This example focuses on the modeling and retrofit design of a municipal wastewater treatment plant. It addresses issues of nutrient removal and it is recommended for users with interests in *industrial and municipal wastewater treatment*.
OJPowder	SuperPro /EnviroPro Designer	This example analyzes a process for producing dehydrated orange juice powder. It is recommended for users with interests in *food processing*.
PharmTbl	SuperPro Designer	This example deals with a process for making pharmaceutical tablets. It is recommended for people that deal with *secondary manufacturing (dosage formulation and fill-finish) of pharmaceuticals and related products*.
SynPharm	SuperPro /EnviroPro Designer	This example deals with a synthetic pharmaceutical process. It is recommended for users in the *pharmaceutical and specialty chemical industries*.
UPWater	SuperPro /EnviroPro Designer	This example deals with water purification (ultra-pure water production) and wastewater treatment at a Semiconductor Manufacturing Facility. Evaluation of recycling options for minimizing city water use and wastewater disposal is included. It is recommended for users with interests in *municipal water purification and wastewater treatment*.
Vial	SuperPro Designer	This example deals with a process that manufactures 5 mL lyophilized vials containing a therapeutic protein. This example is recommended for users interested in *fill-finish steps*.

After installing the application(s) on your computer, you will find all shipped example folders in the 'Examples' subdirectory of the installation directory. Each folder contains one or more SuperPro Designer (.spf) or EnviroPro Designer (.epf) files and a detailed readme (.doc) file that describes the examples contained in that folder.

2.1 DEVELOPING A PROCESS MODEL

The first example of this chapter demonstrates the key initialization and analysis steps for modeling a process with SuperPro Designer. The fundamental steps and analysis features used in this example are the same as the steps and features that would be used during the creation of any other type of process. Therefore, regardless of which type of process you intend to model, reading through the following example should provide you with the knowledge required to model processes on your own. In addition, since this example is a batch process, it serves as a medium for discussing several scheduling issues.

The following files are available for this example in the 'Examples\Misc' directory of SuperPro Designer:

1. *GettingStarted#_#a*: This file represents a simple batch process consisting of a reaction step (Batch Vessel Procedure in a Reactor) and a filtration step (Plate and Frame Filtration Procedure). The mass and energy balances for this process model are solved in equipment 'Design Mode' in order to determine equipment sizing parameters. The development and solution of this process model are described in sections 2.1b Starting a New Process File up to 2.1i Simulating the Process and Viewing the Simulation Results. Furthermore, the specification and analysis of scheduling, equipment utilization and resource tracking information for this process model is described in sections 2.1j Setting the Process Scheduling Information up to 2.1k Viewing Scheduling, Equipment Utilization and Resource Tracking Results.
2. *GettingStarted#_#b*: This file is based on the previous one. The mass and energy balances are now solved for known equipment sizes in equipment 'Rating Mode' in order to analyze throughput and economic information. A throughput and debottlenecking analysis for this process is described in section 2.1l Throughput Analysis and Debottlenecking. Furthermore, the specification and analysis of economic information is described in section 2.1m Cost Analysis and Economic Evaluation.

For continuous processes, the steps that are related to scheduling of operations within unit procedures (see 2.1h Initializing Unit Procedures) and of the entire process (see 2.1j Setting the Process Scheduling Information) do not need to be performed.

2.1a Summary Steps

The steps listed below summarize the process of developing a model with SuperPro Designer. These steps are explained in much greater detail in the remainder of this section (within subsections 2.1b through 2.1n). Furthermore, training videos which describe how to create models from scratch can be found at *http://www.intelligen.com/videos.html*. In particular, the Batch Process Tutorial videos on this webpage correspond to the tutorial described in this chapter.

BRIEF OVERVIEW OF THE MODEL DEVELOPMENT AND ANALYSIS PROCESS IN SUPERPRO DESIGNER:

1. Start a new process file by selecting 'Start a New Process File' in the opening dialog of the program. Alternatively, you may start a new process file later by clicking **New** ( ) on the **Main** toolbar or on the **File** menu of the program.
2. Initialize the process model using the following items of the **Tasks** menu: (a) set the plant operation mode (batch or continuous) using item **Set Mode of Operation**, (b) register pure components using item **Pure Components ▸ Register, Edit/View Properties**, register stock mixtures using item **Stock Mixtures ▸ Register, Edit/View Properties**, and (c) if the plant operation mode is batch, specify recipe scheduling information using item **Recipe Scheduling Information**. You may also want to change the default physical units of the process model using item **Process Options ▸ Physical Units Options** on the **Edit** menu.
3. Build the process flowsheet by adding unit procedures from the **Unit Procedures** menu while in **Select Mode** ( ). Switch to **Connect Mode** ( ) to draw streams and connect the unit procedures.
4. Add operations, such as Charge, Agitation, Batch Heating, Batch Stoichiometric Reaction, etc., to unit procedures. Different unit procedures have different operations available to them. Batch/semi-continuous (cyclical) unit procedures can contain one or more operations, whereas continuous unit procedures are equivalent to unit operations. After the desired operations have been added, initialize all operations and streams.
5. Complete the analysis of the process model using the following commands: (a) solve mass and energy balances and size equipment by clicking **Solve M&E Balances** ( ) on the the **Main** toolbar or on the **Tasks** menu, (b) classify streams into different categories (e.g., raw material, revenue, waste, etc.) using item **Stream Classification** on the **Tasks** menu, and (c) perform costing and economic evaluation calculations by clicking **Perform Economic Calculations** ( ) on the **Main** toolbar or on the **Tasks** menu. Other analyses related to scheduling, throughput, and debottlenecking may optionally be performed.
6. Generate charts and view analysis results using items of the **Tasks**, **Charts** and **View** menus. Generate and view reports using items of the **Reports** menu.

2.1b Starting a New Process File

To open SuperPro Designer after it has been installed, select the program shortcut on the Windows **Start** Menu or double-click the file 'Designer.exe' in the installation directory of the application. The following dialog box will appear by default:

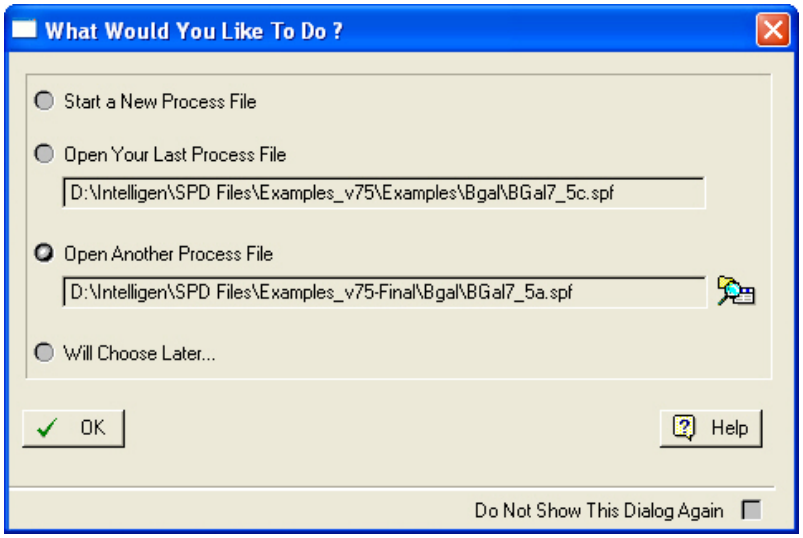


Figure 2.1: The opening dialog box of the program.

To begin working on a new process file, select the option named 'Start a New Process File' from the above dialog and click **OK**. If you select another option and close this dialog, you can always start a new process file later by clicking **New** (🗋) on the **Main** toolbar on the **File** menu.

2.1c Specifying the Mode of Operation for the Entire Plant

After you choose to start a new process file, the 'Process Operating Mode' dialog box will appear as shown in Figure 2.2. This dialog box allows you to set the primary mode of operation (batch or continuous) and the annual operating time available for the entire process. You can also modify these settings at a later time by clicking **Set Mode of Operation** on the **Tasks** menu.

When the process operating mode is set to 'Batch', all stream flows are displayed on a per-batch basis. On the other hand, when the process operating mode is set to 'Continuous', all stream flows are displayed on a per-hour basis. Moreover, no scheduling information is necessary for plants operating continuously.

Please note that although the plant operation mode can be either batch or continuous, SuperPro Designer can also model processes that operate in mixed modes. That is, you can have continuous unit procedures in a batch process plant as well as batch/semi-continuous (cyclical) unit procedures in a continuous process plant. This is explained later in this chapter (see 2.1h Initializing Unit Procedures).

For now, let's select 'Batch' as the operating mode of this example process and click **OK**.

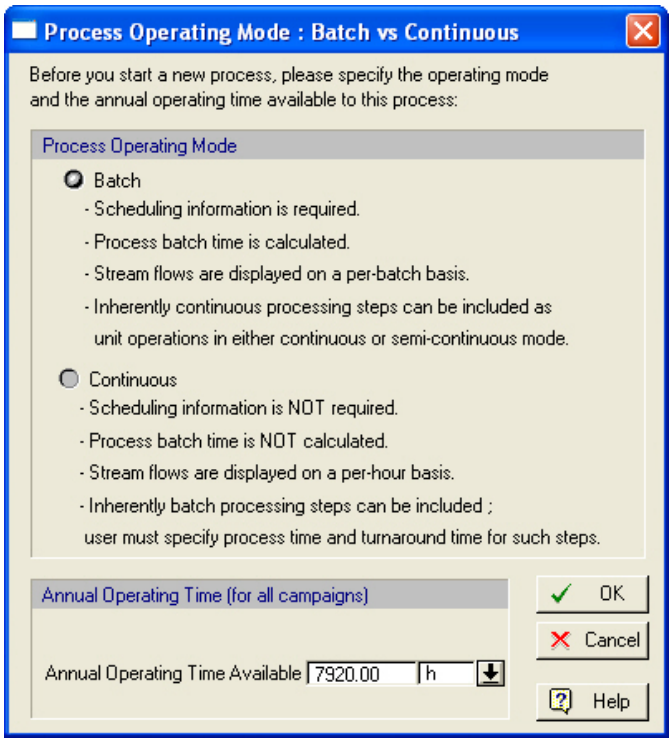

Process Operating Mode : Batch vs Continuous
Before you start a new process, please specify the operating mode and the annual operating time available to this process:
Process Operating Mode
Batch
- Scheduling information is required.
- Process batch time is calculated.
- Stream flows are displayed on a per-batch basis.
- Inherently continuous processing steps can be included as unit operations in either continuous or semi-continuous mode.
Continuous
- Scheduling information is NOT required.
- Process batch time is NOT calculated.
- Stream flows are displayed on a per-hour basis.
- Inherently batch processing steps can be included ; user must specify process time and turnaround time for such steps.
Annual Operating Time (for all campaigns)
Annual Operating Time Available
7920.00
h
OK
Cancel
Help

Figure 2.2: The 'Process Operating Mode' dialog box.

2.1d Setting the Default Physical Units

SuperPro Designer provides a variety of options for units of measure for the entry and display of data. To view or modify the default units of the process model, click on an empty area in the flowsheet and then select **Process options ▸ Physical Units Options** from the **Edit** menu. Alternatively, right-click on the flowsheet to bring up its context menu and select **Physical Units Options**.

*To activate the **Process Options** menu item on the **Edit** menu, you must first click on an empty area of the flowsheet.*

2.1e Registering Components and Mixtures

COMPONENT DATABANKS

SuperPro Designer's component databank provides for the use of multiple source databases. The following databases can be used to provide component-related properties:

- the 'Designer' database,
- the 'User' database,
- the DIPPR database, and

- the PPDS database.

Each database is contained in a separate file. The 'Designer' component database is part of the 'Designer' (or 'System') database; it provides data for over 530 commonly used compounds.

The 'User' component database is part of the 'User' database, and it is a repository available for users to store data for their own (or 'user-defined') components. The 'User' component database is originally empty (upon installation of the software).

The DIPPR database draws its data from the relational form of the DIPPR collection of component data. This component database was developed at Brigham Young University, although it is now licensed by AIChE (see *http://www.aiche.org/dippr*). A demo version of the DIPPR database with only 5 components is shipped and installed with SuperPro Designer.

The PPDS database is licensed by TÜV SÜD (see *http://www.tuv-sud.co.uk/uk-en/about-tuev-sued/tuev-sued-in-the-uk/nel/ppds-thermodynamic-properties-suite*), and it provides pure component physical property data and binary coefficients for a wide range of applications.

To change the location of the database files, click **Availability, Passwords and Locations** on the **Databanks** menu to display the Databases: Availability, Password & Locations Dialog. For example, if the full DIPPR database is available or if you want to use a different 'User' database file based on a file that somebody else created, you must specify its location through that dialog; for more details, see 15.1 Database Registration.

REGISTERING COMPONENTS

All the components that will be used in a process model must be registered first. To register components (in other words, to make them available in your process model), select **Pure Components ▸ Register, Edit/View Properties** on the **Tasks** menu. This will activate the dialog shown in Figure 2.3.

Note that pure components 'Nitrogen', 'Oxygen', and 'Water' are registered by default in every new process model and cannot be deleted. For this example process, you will need to add 'Heptane' to the list of registered pure components (shown on the RHS of this dialog) as well. To add 'Heptane', you can either scroll down to it in the list of available pure components in the 'Designer' database (shown on the LHS of this dialog), or you can begin typing "heptane" in the box above the list (as shown in Figure 2.3) and the database will automatically scroll to the correct location. Next, click **Register** ( ) to add 'Heptane' to the list of registered pure components for this process model. Alternatively, you may double click on 'Heptane' in the database listing and it will be added to your list of registered components.

If a component is not available in the existing component libraries, you can click **New** () on the 'Registered Pure Components' toolbar to create a new component for your process model. This will be automatically added to the list of registered components. For this process, you will need to create components 'A', 'B', and 'C'. These components will represent the reactants and product of a simple reaction.

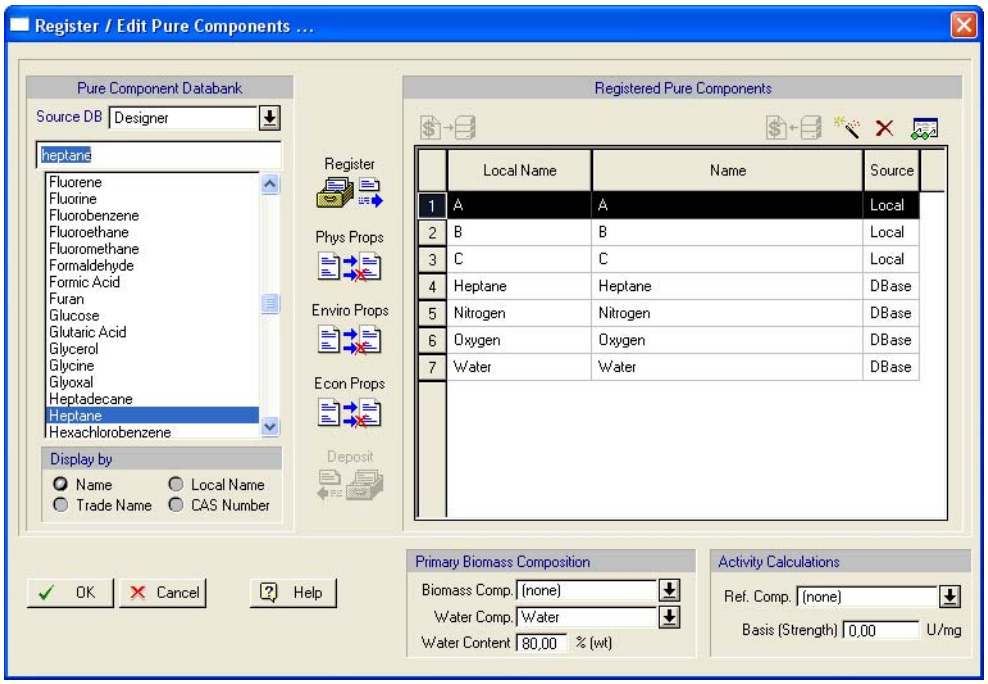


Figure 2.3: The pure component registration dialog box.

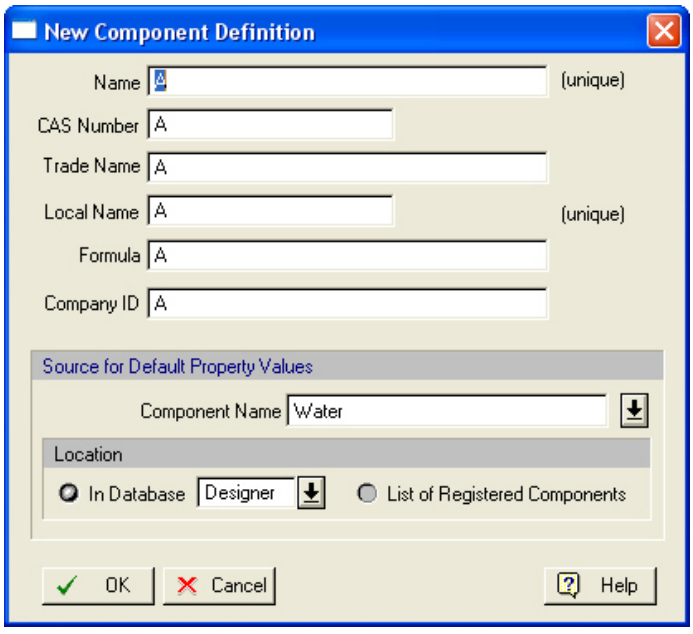


Figure 2.4: The 'New Component Definition' dialog box.

To create component 'A', click **New** ( ) and in the 'New Component Definition' dialog that appears (see Figure 2.4) fill-in the letter "A" for the 'Name' field. Notice that as you type, the contents of the 'Name' field are automatically copied to all other fields ('CAS Number', 'Trade Name', 'Local Name', 'Formula', and 'Company ID').

As far as the program is concerned, you do not need to have correct CAS Numbers, Formulas, etc. You just need to have something written in each of these six fields. The 'Local Name' is the one that appears in the reports and all the input/output dialog windows of the program.

Notice that at the bottom of this dialog, you can choose to initialize the properties of the new component by copying them from some other database component or registered component. For this example, click **OK** to copy the properties of component 'Water' (which is available in the 'Designer' database) to component 'A'.

After you have added component 'A' to your list of registered components, follow the same steps to add components 'B' and 'C'. When you have completed this, you should edit some of the properties of these components. To access the properties of component 'A', double-click on that component in the list of registered pure components. Alternatively, you can highlight the component (by clicking on it once) and then click the **Properties** button ( ) on the 'Registered Pure Components' toolbar. This will bring up the 'Pure Component Properties' dialog box for component 'A'. Through this dialog you can view or edit a component's physical and environmental properties, cost data, and regulatory information.

For the purposes of this example, the only physical parameter we will be concerned with is the molecular weight (MW). Please go to the 'Physical (Constant)' tab and change the MW of component 'A' to 150 g/gmol as shown in Figure 2.5. Also, visit the 'Economics' tab and specify a purchasing price of $10/kg. Then click **OK** to close the dialog.

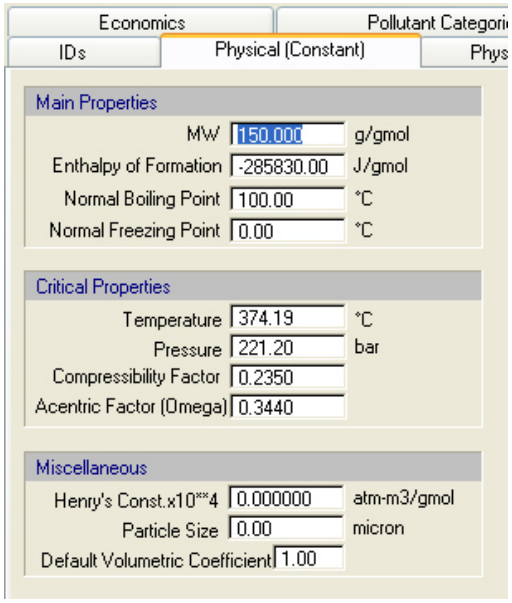


Figure 2.5: Editing the constant physical property values of component 'A' in the example.

Next, please visit the properties dialog for component 'B' and enter a MW of 25 g/gmol and a purchasing price of $15/kg. Also, visit the properties dialog for component 'C' and enter a MW of 175 g/gmol and a selling price of $200/kg. This completes your initialization of components for our simple example. Click **OK** on the pure component registration dialog box to save your changes.

To delete a registered pure component, highlight that component in the list of registered pure components and click **Delete** *(✕) on the 'Registered Pure Components' toolbar.*

You can add a registered pure component which you have created or modified in your process file to the User databank. This will allow you to register that same component in other files as well (rather than having to manually re-create the component in other files). To add a component to the User databank, first select 'User' in the 'Source DB' drop-down list. Then highlight the registered component and click on the **Deposit** *button:*

The current version of SuperPro Designer does not make use of the Normal Freezing Point of pure components. The corresponding field entry, which can be found in the 'Physical (Constant)' tab of the 'Pure Component Properties' dialog, can be ignored.

REGISTERING MIXTURES

Mixtures are used to facilitate initialization of input streams in cases where certain raw materials (e.g., buffers) are consumed as mixtures. In order to register a mixture, click Stock Mixtures ▸ Register, Edit/View Properties on the Tasks menu and follow the same steps as for registering pure components. Note that many of the specifications related to stock mixtures differ from the specifications for pure components. For more information on stock mixture specifications, see 3.2 Stock Mixtures.

2.1f Saving and Opening Files

At this point, please save your file by clicking **Save As** from the **File** menu and giving your process model a descriptive name in the Windows 'Save As' dialog box that appears. In general, it is a good idea to save your work often in order to avoid having to redo work in the event of a program crash.

When working with larger process files, include the date or some other version indicator in the saved case name.

If the program does crash, there is sometimes a possibility that you will not be able to re-open the file you were most recently working on. In that case, you should try to open the backup versions of your file. Anytime you save a newer version of your file, SuperPro Designer will also save a backup copy of the previous version using file extension '.sp~' (as opposed to a normal '.spf' file). If the '.sp~' backup file already exists, SuperPro Designer will first create a copy of that file using file extension '.s~~' as a second backup.

To open a file, click **Open** from the **File** menu. This will bring up the Windows 'Open' dialog box. To open a backup file, simply go to the directory where you saved your original file, select

the corresponding '.sp~' or '.s~~' backup file (select 'All Files (*.*)' in the 'File Type' field of the dialog box) and click the **Open** button.

Note that the corresponding file extensions for the original, backup, and second backup files in EnviroPro Designer are '.epf', '.ep~' and '.e~~'..

*SuperPro Designer allows projects to be saved automatically at specific time intervals. To activate the auto-save functionality, first select **Application Settings** from the **File** menu. On the dialog that appears, click-on the **Auto-Save** checkbox and then specify the time interval.*

2.1g Building the Process Flowsheet

ADDING UNIT PROCEDURES

The first step in building a flowsheet is to add processing steps (unit procedures) to the process. A unit procedure is defined as a series of operations that take place within a piece of equipment. The types of operations available depend on the type of unit procedure you are using. As explained later in this chapter (see 2.1h Initializing Unit Procedures), batch/semi-continuous (cyclical) unit procedures can contain one or more operations, whereas continuous unit procedures are equivalent to unit operations.

To add a unit procedure to the flowsheet, first select the desired unit procedure from the **Unit Procedures** menu. For our example, please select **Batch Vessel Procedure ▸ in a Reactor**. Notice that after you select a unit procedure and move the mouse pointer to the flowsheet area, it changes to the 'add step' pointer ( ). This indicates that your next mouse click on the flowsheet will lay down the icon of the selected unit procedure in that location. Please click near the left side of the flowsheet to lay down the icon of the selected unit procedure. SuperPro Designer automatically adds a default procedure name ('P-1'), host equipment name ('R-101') and procedure description ('Vessel Procedure') below the icon..

*If you decide to abort the addition of the new unit procedure, you can simply hit the **Esc** key on your keyboard.*

*If you wish to modify the default equipment name prefixes (e.g. 'R' for a Stirred Reactor (CSTR) vessel and 'PFF' for a Plate & Frame Filter), click **Application Settings** on the **File** menu and go to the 'Prefixes' tab. To edit the prefix of an equipment resource, highlight that equipment in the available list and click on the corresponding prefix. Through the same tab, you can also modify the default operation prefixes in the same manner; for more details, see 8.20 Application Settings.*

After you have added a Batch Vessel Procedure in a Reactor to the flowsheet, please add a Plate and Frame Filtration Procedure by clicking **Filtration ▸ Plate and Frame Filtration** on the **Unit Procedures** menu and then clicking somewhere to the right of the vessel procedure icon. Your flowsheet should now look something like this:

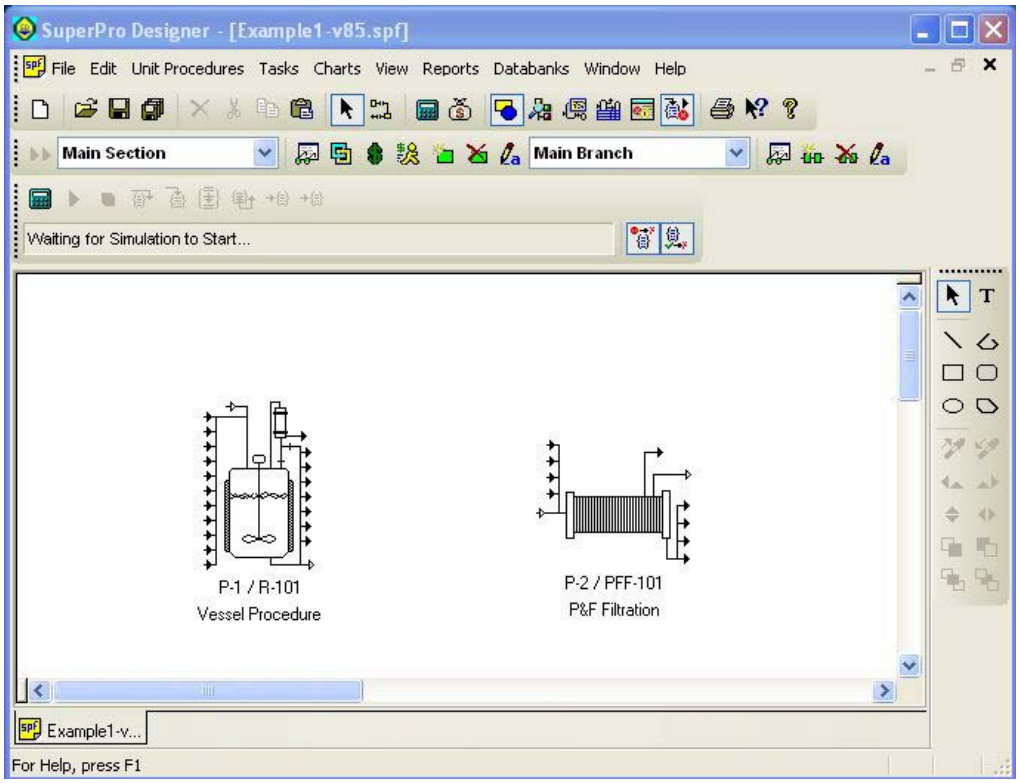


Figure 2.6: The example process with the Batch Vessel Procedure in a Reactor and Plate and Frame Filtration Procedure icons added

Moving, Copying and Deleting Unit Procedures

The following guidelines show how you can move or delete unit procedures in a flowsheet, and how you can cut or copy and paste unit procedures to a different location in the same flowsheet or in another flowsheet.

First, you need to select the desired unit procedure icon(s). You can select a single icon by clicking on it. You can select multiple icons by either dragging an enclosing rectangle around them, or by adding icons to the selection. To add an icon to the selection, click on it while holding down the **Ctrl** key. To remove an icon from the selection, **Ctrl+Click** on it again. To select an entire flowsheet, click **Select All** on the **File** menu or press **Ctrl+A**.

▶ To Move Unit Procedures...

1. Select the desired unit procedure icon(s).
2. Drag the selected icon(s) to the new location. If multiple icons are selected, you can drag any member of the selection and all icons will move simultaneously. You can use the arrow keys to move the selection one pixel at a time.

Note that when you move a unit procedure icon that has streams attached to it, all streams will move with it. If two unit procedures are connected through an intermediate stream and both the source and destination unit procedures move, then the stream will keep its structure intact and move with them. If one of the stream's ends remains anchored while the other end is being moved, then the stream will adjust its first and/or last elbow to accommodate the change of location; for more details on streams, see 'Adding Streams' on page 2-15.

▶ To Delete Unit Procedures...

1. Select the desired unit procedure icon(s).
2. Hit the **Delete** key on your keyboard or click **Clear** on the **Edit** menu. The selected unit procedure(s) will be erased.

When you delete a unit procedure, all streams attached to it will also be deleted.

▶ To Cut or Copy and Paste Unit Procedures...

SuperPro Designer allows you to cut or copy unit procedures into the clipboard so that you can subsequently paste them to a different location, either in the same flowsheet or in another flowsheet. To do this:

1. Select the desired unit procedure icon(s).
2. To cut the icon(s), click **Cut** on the **Edit** menu (or press **Ctrl+X**). To copy the icons, click **Copy** on the **Edit** menu (or press **Ctrl+C)**.
3. Move the mouse cursor to the desired area in the same flowsheet or in another flowsheet and click **Paste** on the **Edit** menu (or press **Ctrl+V**) to paste the icon(s).

The following restrictions apply to the use of the Cut, Copy and Paste features:

1. You cannot cut or copy and paste streams alone. Streams are placed onto the clipboard only if you use the mouse to drag an enclosing rectangle around the unit procedure(s) and its associated streams.
2. When pasting unit procedures into a flowsheet, you should be aware that certain features of the original unit procedures are *not transferred* into the newly created copy:

   (a) When you cut or copy a single unit procedure (without also selecting its attached streams), the attached streams are not included in the pasted set.

   (b) If the start time of the first operation of the pasted unit procedure was defined on a relative basis (e.g., with respect to the start or end of another operation in some other procedure), then the scheduling of the pasted procedure is reset to remove the coupling.

   (c) If the original unit procedure was sharing equipment with another procedure, the pasted procedure is reset to be executed in its own equipment.

3. Pasting streams and certain processing steps with component- and stock mixture- related specifications from one flowsheet to another is not possible unless all components and stock mixtures of the source process model exist in the destination process model as well. If

that is not the case, the program will automatically expand the set of registered pure components and stock mixtures in the destination process to include the missing ones.

If you want to paste icons from the flowsheet into another application (e.g., a word processing application), please consult Chapter 14 (Exchanging Data with Other Apps).

Accessing the Help Files

In many equipment resources that host unit procedures, there are dedicated ports, such as 'Feed', 'Vent (Emissions)', 'Cake Removal', 'Filtrate Removal', etc. *These ports may only be used by certain types of streams*. To see which ports are dedicated to each function, you

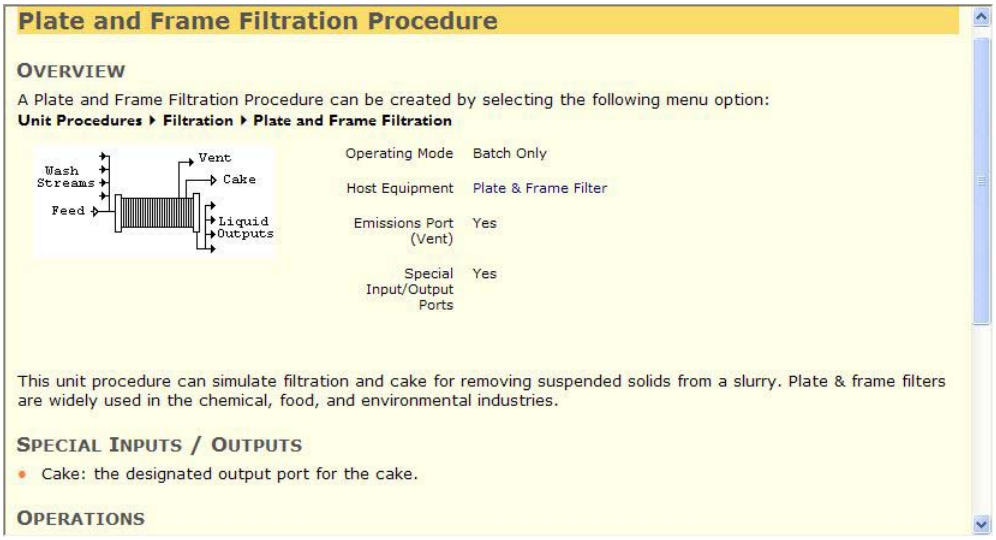


Plate and Frame Filtration Procedure
OVERVIEW
A Plate and Frame Filtration Procedure can be created by selecting the following menu option:
Unit Procedures ▸ Filtration ▸ Plate and Frame Filtration
Wash Streams
Feed
Vent
Cake
Liquid Outputs
Operating Mode Batch Only
Host Equipment Plate & Frame Filter
Emissions Port (Vent) Yes
Special Input/Output Ports Yes
This unit procedure can simulate filtration and cake for removing suspended solids from a slurry. Plate & frame filters are widely used in the chemical, food, and environmental industries.
SPECIAL INPUTS / OUTPUTS
Cake: the designated output port for the cake.
OPERATIONS

Figure 2.7: The help topic for the Plate and Frame Filtration Procedure.

can look up the desired equipment or unit procedure in the program's Help system, which is available through the **Help** menu. This provides access to supporting documentation shipped with the software, such as the electronic version of the User's Manual and additional content.

As a shortcut to the **Help** menu for any unit procedure, you can click **Help** ( ) on the **Main** toolbar and then click on the unit procedure icon you are interested in. Alternatively, you can click on the unit procedure icon and hit the **F1** key. Note that you can also use the **Help** ( ) button feature as a shortcut to access the Help files for other interface elements, such as menu options, toolbar buttons, dialog boxes and dialog tabs.

At this point, please open the Help file for the Plate and Frame Filtration Procedure. A portion of that file is shown in Figure 2.7. Notice that dedicated ports of the host equipment (Plate & Frame Filter) are labeled next to its icon. The Help file for each unit procedure also contains a general description, links to its operation models and to the host equipment, and much more.

ADDING STREAMS

After you add a unit procedure to the process flowsheet, you can add streams. There are three types of streams:

- feed (input) streams,
- intermediate streams, and
- product (output) streams.

Feed (input) streams do not have a source unit procedure and in batch processing they are mainly utilized by charge operations. Intermediate streams connect two unit procedures and they are used to transfer material from the source to the destination unit procedure. Product (output) streams do not have a destination unit procedure. All streams are automatically identified with a stream tag.

In order to add streams to the flowsheet, you must first click **Connect Mode** ( ) on the **Main** toolbar. When you do this and return to the flowsheet, the mouse pointer changes to the 'add stream' pointer ( ) to indicate that you are in 'Connect Mode' (as opposed to 'Select Mode'). Then you can add feed, intermediate, and product streams as described below:

▶ To Add a Feed Stream...

1. Click on an empty area in the flowsheet to initiate drawing of the stream. Notice that as you move the mouse pointer over the inlet and outlet ports, it changes to a 'port' pointer ( ).
2. Move the mouse pointer over the desired inlet port of the destination unit procedure and once the 'port' pointer is displayed click on the port to terminate the stream line. SuperPro Designer automatically draws the feed stream symbol at the beginning of the stream and labels the stream.

▶ To Add an Intermediate Stream...

1. Move the mouse pointer over the desired outlet port of the source unit procedure and once the 'port' pointer is displayed click on the port to initiate drawing of the stream.
2. Move the mouse pointer over the desired inlet port of the destination unit procedure and once the 'port' pointer is displayed click on the port to terminate the stream line. SuperPro Designer automatically labels the stream.

▶ To Add a Product Stream...

1. Move the mouse pointer over the desired outlet port of the source unit procedure and once the 'port' pointer is displayed click on the port to initiate drawing of the stream.
2. Double-click on an empty area of the flowsheet to terminate the stream. SuperPro Designer automatically draws the product stream and labels the stream.

Note that between initiation and termination of a stream, you may optionally click at intermediate points on the screen to create right angle bends. This permits customizing of the stream route and flexibility in flowsheet design. You can cancel the stream-drawing process at any time by simply hitting the Esc key on your keyboard. Then you can restart the stream-drawing process by clicking **Connect Mode** ( ) again on the **Main** toolbar. To delete a stream, simply select it (by clicking on it) and press the **Delete** key on your keyboard.

At this point, please add the feed, intermediate, and product streams to your example process. Your flowsheet should now look like the one shown in Figure 2.8:

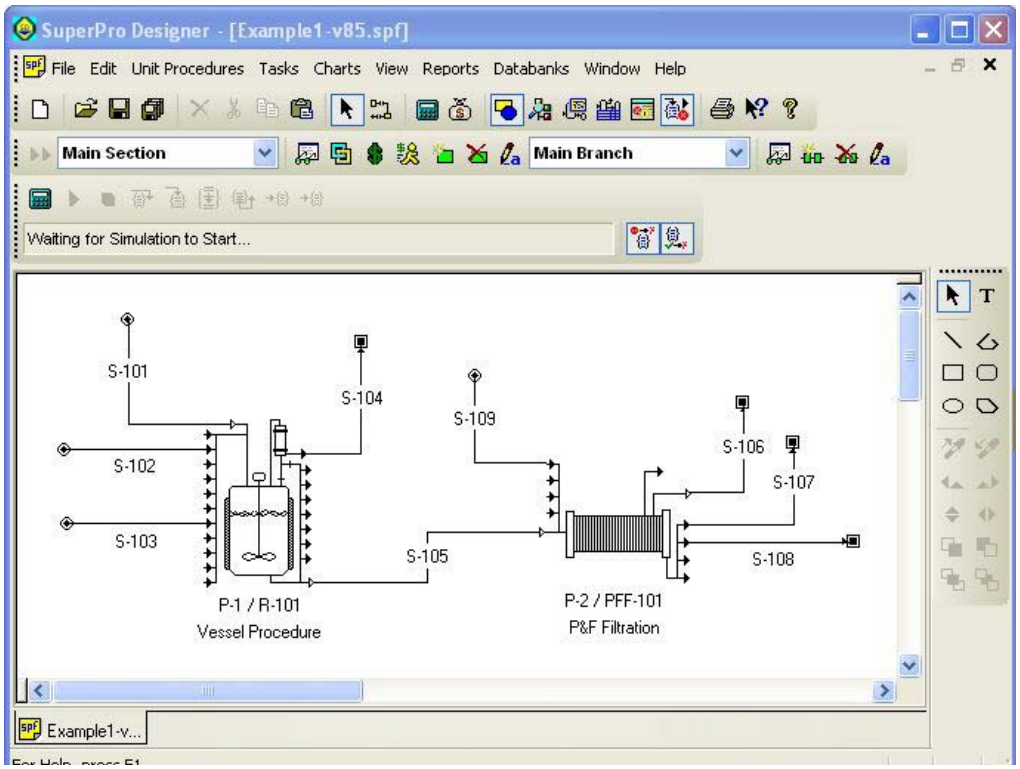


Figure 2.8: The example process flowsheet with streams added.

Changing the Appearance of Streams

When SuperPro Designer is in 'Select Mode' and the mouse pointer is over a stream line, it changes to a 'menu' pointer ( ) to indicate the availability of a stream context menu (see Figure 2.9). This menu can also be displayed by right-clicking on a stream line.

Through the stream context menu, you can view or edit (in the case of input streams) the composition, flowrate, and other stream properties using item **Simulation Data**, select different stream initialization options using item **Initialization Options**, change the tag name (label) of the stream using item **Edit Tag Name**, adjust the elbows of the stream line using item **Edit Elbows**, edit the stream style (e.g., label and line color, line thickness, etc.) using item **Edit Style**, etc. Note that double-clicking on a stream line is equivalent to clicking **Simulation Data** on the stream's context menu.

At this point, please right-click on input stream 'S-101' of the vessel procedure 'P-1' and click **Edit Tag Name** on the stream's context menu. Change the name of the stream to 'Heptane' and click **OK**. Then, right-click on the 'Heptane' stream line and click **Style ▸ Edit Style** to display the 'Stream Style' dialog.

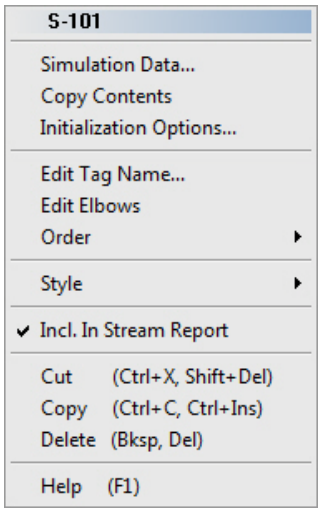


Figure 2.9: The stream context menu.

In the 'Stream Line' tab of this dialog (see Figure 2.10), click **Pen Color** ( ) on the 'Stream Line' toolbar and change the color to blue. Also click **Pen Size** ( ) on the same toolbar and change the size to 2 pixels.

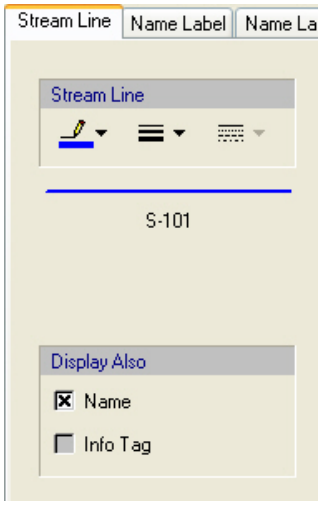


Figure 2.10: The 'Stream Line' tab of the 'Stream Style' dialog box.

Now, switch to the 'Name Label' tab. Click **Font Color** ( ) on the 'Color / Font' toolbar and change the color to teal. Also, click **Font** ( ) on the same toolbar and change the font style to bold and the font size to 12. Then click the 'Name Label: Location' tab, change the segment preference to 'Vertical Near Source' and click **OK**.

Next, please change the name of stream 'S-106' (the stream that is connected to the dedicated cake removal port of the Plate & Frame Filter) to 'Cake'. Also, apply the style of the 'Heptane'

stream to the 'Cake' stream and to the intermediate stream 'S-105' using the shortcut method described below:

▶ To Apply the Style of a Stream to Several Other Streams...

1. Right-click on the source stream line (e.g., the 'Heptane' stream in the example) and click **Style ▸ Pickup Style**.
2. Right-click on the desired target stream line(s) (e.g. the 'Cake' and 'S-105' streams in the example) and click **Style ▸ Apply Style**.

After applying these changes, your streams should look something like this:

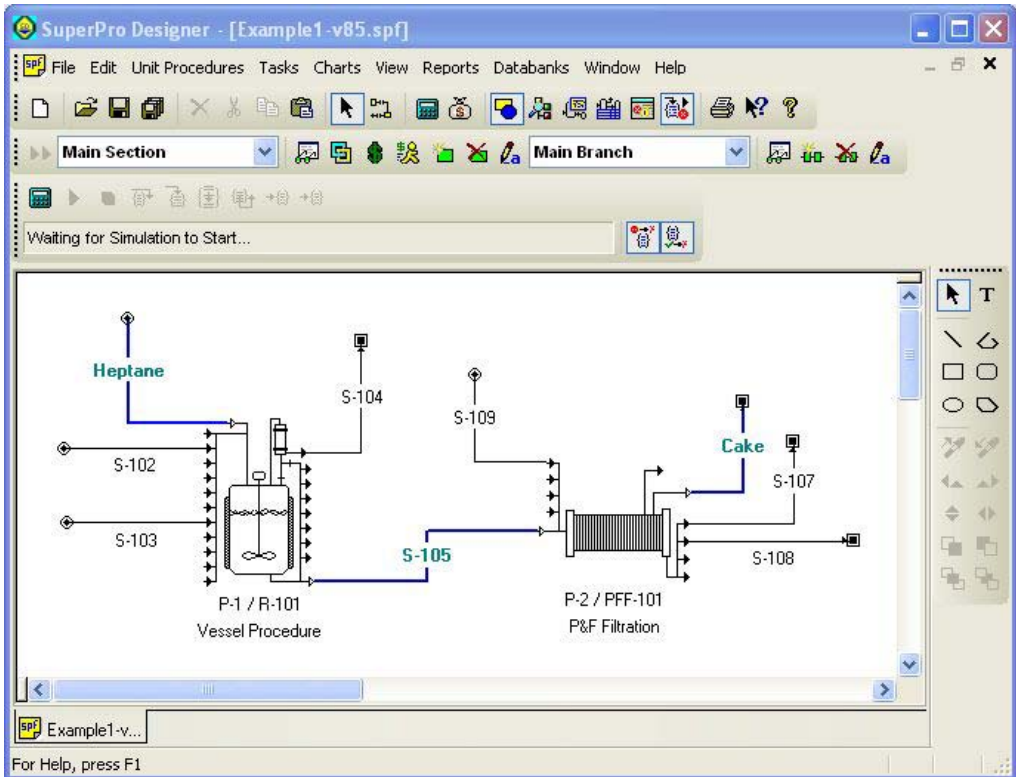


Figure 2.11: The example process flowsheet after the names and styles of streams have been changed.

For more information on stream drawing, see 4.10 Classification of Input and Output Streams.

2.1h Initializing Unit Procedures

SPECIFYING THE OPERATING MODE OF UNIT PROCEDURES

Each unit procedure added to the process has its own operating mode setting. This can be either:

- batch/semi-continuous, or
- continuous.

Batch/semi-continuous (cyclical) unit procedures can contain one or more operations, whereas continuous unit procedures are equivalent to unit operations. There are unit procedures that are inherently batch/semi-continuous (e.g., the Batch Vessel Procedure in a Reactor employed in this example) and can only be operated in batch/semi-continuous mode. You can have batch/semi-continuous unit procedures in continuous process plants. Other unit procedures are inherently continuous (e.g., the Centrifugal Pumping unit procedure which is available by clicking **Transport (near)** ▸ **Liquids** ▸ **Centrifugal Pump** on the **Unit Procedures** menu). By default, these can be operated in either mode. Thereby, you can have continuous unit procedures in batch process plants. Note that the operating mode of inherently continuous unit procedures is initially set to batch/semi-continuous in batch process plants and continuous in continuous process plants.

You can access or modify (where both options are available) the operating mode of a unit procedure through its context menu. Please right-click on a unit procedure icon on your flowsheet to bring up its context menu. The context menu of vessel procedure 'P-1' is shown in Figure 2.12. To view the operating mode setting of a unit procedure, click **Procedure Data**. This will display the 'Procedure Data' dialog for that unit procedure. The operating mode specifications can be found in the 'Scheduling' tab of that dialog; for more details on the operating mode of unit procedures, see Chapter 5 (Procedures & Operations).

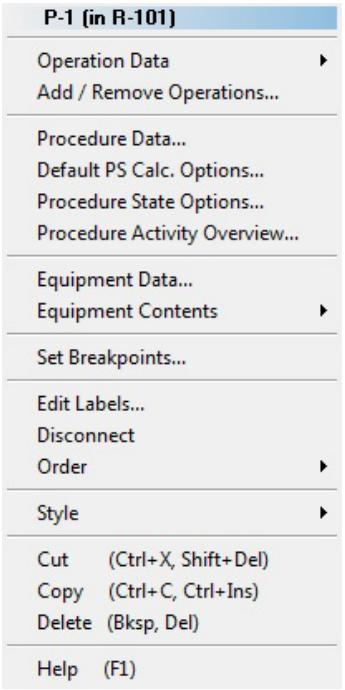


Figure 2.12: The context menu of the Batch Vessel Procedure in a Reactor in the example.

The meaning of each item in the context menu of a unit procedure is explained below:

- The **Operation Data** item allows you to access or modify the simulation parameters of the operations that have been added to the unit procedure. Note that this item is not available if no operations have been added to the unit procedure. If the unit procedure

contains a single operation, clicking on this menu item will bring up the 'Operation Data' dialog for that operation. If it contains more than one operations, clicking on this menu item or simply moving the mouse pointer over it will bring up a drop-down list of all added operations. Clicking on an operation in that list will bring up its 'Operation Data' dialog.

- The **Add/Remove Operations** item allows you to add/remove operations to/from the unit procedure and change the sequence in which these operations are executed. This item is only available for unit procedures that are operated in batch/semi-continuous mode.
- The **Procedure Data** item allows you to access or modify the simulation parameters of the unit procedure, such as the operating mode (continuous or batch/semi-continuous) as well as additional scheduling, throughput analysis and debottlenecking information.
- The **Default PS Calc Options** item allows you to set the default physical state properties of pure components for all operations in the procedure. Note that it is also possible to globally-specify the default physical state options for all procedures in the flowsheet by right-clicking an open area of the flowsheet, selecting the **PS Calculation Options** menu, and specifying the desired shortcut or rigorous options in the relevant sub-menu.
- The **Procedure State Options** item allows you to access or modify physical state properties of pure components during each individual operation. Specifications made in this dialog will override the default specifications set in the **Default PS Calc Options** dialog. For more information on the selection of physical state options, please refer to chapter 8.12 Physical State Calculation Options.
- Through the **Procedure Activity Overview** item, you can view a summary of scheduled operations, processed material, and equipment contents during the execution of the unit procedure.
- The **Equipment Data** item allows you to access or modify the simulation parameters of the host equipment, such as sizing, costing, and scheduling information.
- The **Equipment Contents** item allows you to access or modify the initial equipment contents, and also view a summary of the thermodynamic properties and composition of the equipment contents during the execution of the unit procedure.
- The **Set Break Points** item allows you to place stops in the sequential solution of mass and energy balances. This is normally used for troubleshooting in large or complex process simulations.
- The **Edit Labels** item allows you to change the name of the unit procedure, the name of the host equipment and the description of the unit procedure. For example, you can change the default unit procedure name ('P-1'), equipment name ('R-101') and unit procedure description ('Vessel Procedure') for the vessel procedure in this example.
- The **Disconnect** item deletes all streams connected to the unit procedure.

- The **Flip (reverse flow direction)** item allows you to change the flow direction of the unit procedure icon from left-to-right (default) to right-to-left and vice versa. You can also do that by clicking **Flip Horizontally** ( ) on the **Visual Objects** Toolbar (see 13.5 Visual Objects Toolbar). Note that this option is only available when the unit procedure does not have any streams attached to it.
- The **Order** item forces the unit procedure icon to appear behind or in front of other icons, text, etc.
- The **Style** item allows the user to edit such things as the icon color, the tag name color and font, etc.
- The **Cut**, **Copy**, and **Delete** items perform the tasks described by their names.
- The **Help (F1)** item provides access to the Help file of the unit procedure.

ADDING OPERATIONS TO UNIT PROCEDURES

The next step toward initialization of unit procedures is to add relevant operations to each unit procedure. This step is generally required for unit procedures that are operated in batch/semi-continuous mode. For convenience, some inherently batch/semi-continuous unit procedures may initially contain one or more operations when added to the process (e.g., the Plate and Frame Filtration Procedure used in this example initially has a Cloth Filtration operation). An equivalent operation is always added to unit procedures that are inherently continuous, when these are added to the process (e.g., the Centrifugal Pumping unit procedure will contain a Centrifugal Pumping operation).

In order to add operations to a unit procedure that is operated in batch/semi-continuous mode, you can either:

- double-click on a unit procedure icon, or
- right-click on the unit procedure icon and select **Add / Remove Operations** from the context menu of that unit procedure. Note that this menu item is only available for unit procedures that are operated in batch/semi-continuous mode.

Either action will bring up the 'Operation Sequence' dialog (see Figure 2.13) for the selected unit procedure.

Double-clicking on a continuous unit procedure (e.g., a Centrifugal Pumping unit procedure added to a continuous process plant) brings up the dialog window of its operation instead of the 'Operation Sequence' dialog. Essentially, a unit procedure that is operated in continuous mode behaves like a single operation.

At this point, please open the 'Operation Sequence' dialog for the vessel procedure ('P-1') in the example. Add a Charge operation to the operation sequence for this unit procedure by double-clicking this item in the list of available operations. Alternatively, you can highlight this item and click **Add** ( ) to add the new operation at the end of the operation sequence or **Insert** ( ) to insert the new operation *before* the highlighted operation in the operation sequence. To delete an operation from the operation sequence, select it and click **Delete** ( ) on the available toolbar. If you add an operation in the wrong order, you can change its position in the operation sequence using the **Move Up** ( ), **Move Down** ( ), **Move to Top** ( ), and **Move to Bottom** ( ) buttons on the same toolbar.

Notice that the charge operation is initially named ‘CHARGE-1’ when it is added to the operation sequence. Double-click that item (or highlight that item and click **Rename** ( ) on the available toolbar) and change the name of the added charge operation to ‘Charge Solvent’. Now, add two more Charge operations, a ‘React (Stoichiometric)’ (Batch Stoichiometric Reaction) operation, and a Transfer Out operation, to the operation sequence. Rename these operations to ‘Charge Reactant A’, ‘Charge Reactant B’, ‘React’ and ‘Transfer to PFF-101’, respectively, so that your dialog box looks like the one shown in Figure 2.13. Then click **OK** to return to the process flowsheet.

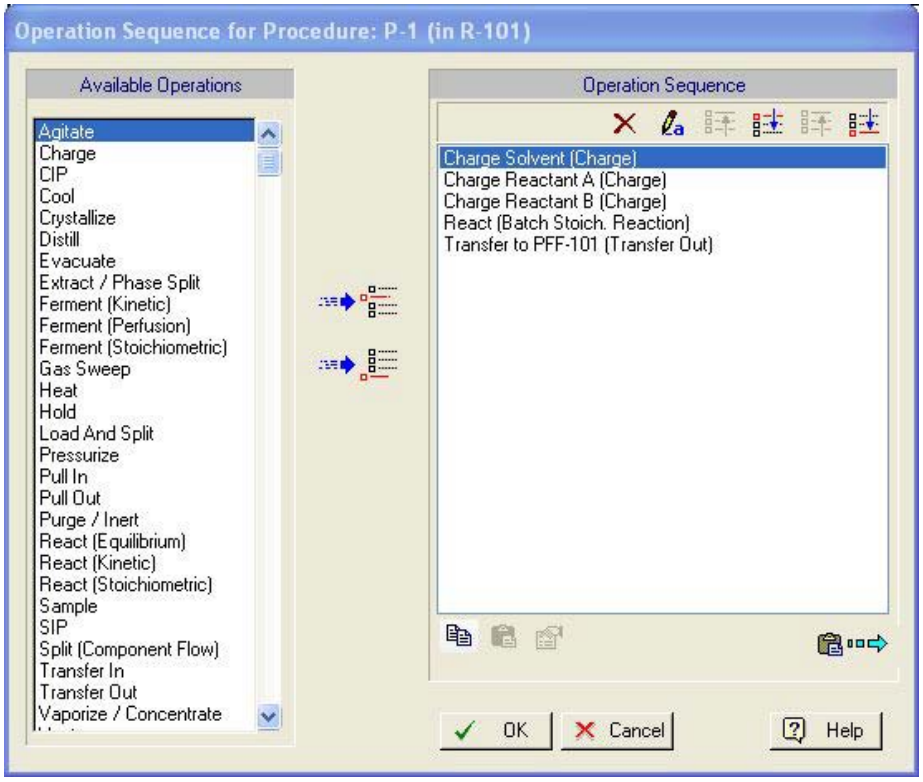


Figure 2.13: Adding operations to the Batch Vessel Procedure in a Reactor in the example.

Subsequently, please open the ‘Operation Sequence’ dialog for the filtration procedure (‘P-2’) in the example. Notice that this unit procedure has a ‘Filter’ (Cloth Filtration) operation (named ‘FILTER-1’) added to its operation sequence by default. Use the same method as before to add a ‘Wash Cake’ (Cake Wash) operation (named ‘CAKE-WASH-1’) and a Transfer Out operation (named ‘TRANSFER-OUT-1’) to the operation sequence. You can keep the default names for these operations.

INITIALIZING THE OPERATIONS

The next step is to initialize the operations added to the two unit procedures as described below.

Batch Vessel Procedure in a Reactor

Please right-click on the vessel procedure ('P-1') to bring up its context menu and click **Operation Data ▸ Charge Solvent (Charge)**. This will bring up the 'Operation Data' dialog for the 'Charge Solvent' operation. Through this dialog, you can access or modify the simulation data for an operation, such as the operating conditions, scheduling data, emission specifications, and labor-related information. This data is grouped into several tabs. Note that different tabs may be available for different operations. The operating conditions ('Oper. Cond's') tab for the 'Charge Solvent' operation of this example is shown in Figure 2.14

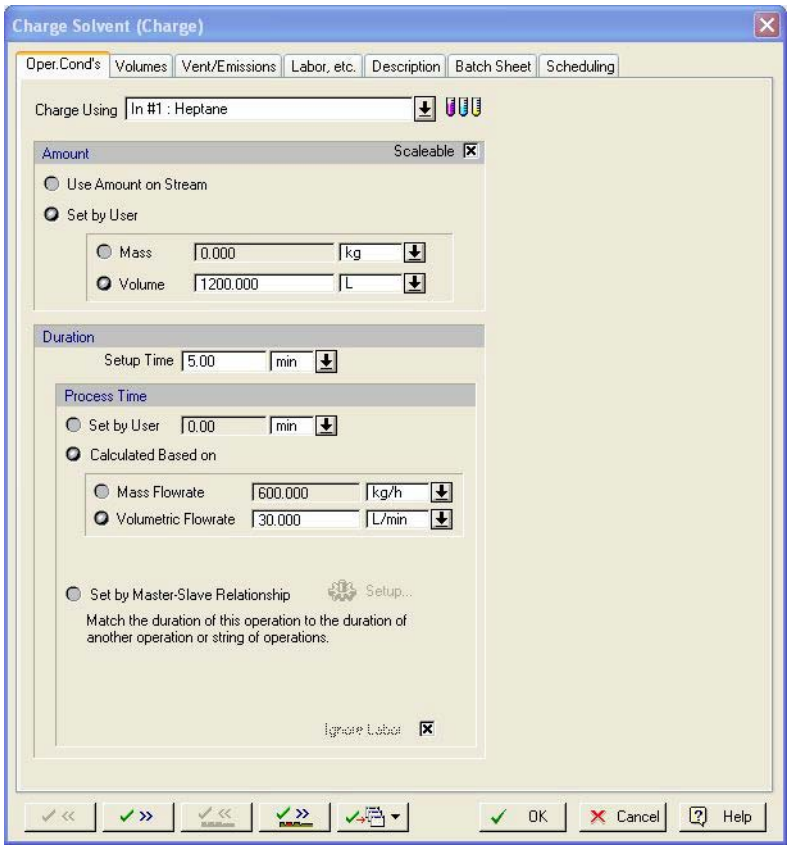


Figure 2.14: The 'Oper. Cond's' tab for the first Charge operation ('Charge Solvent') in procedure 'P-1'.

To initialize the operating conditions for the 'Charge Solvent' operation, you begin by selecting the charge stream for this operation. Use the 'Charge Using' drop-down list at the top of the tab to select the stream which you renamed 'Heptane' earlier in this section. Then click on the **View/Edit Stream Composition and/or Amount** ( ) button next to the drop-down list in order to access the simulation data dialog for that stream (see Figure 2.15) and specify its

composition. To add ‘Heptane’ to the stream, double-click on the corresponding item in the ‘Registered Ingredients’ listing for that stream.

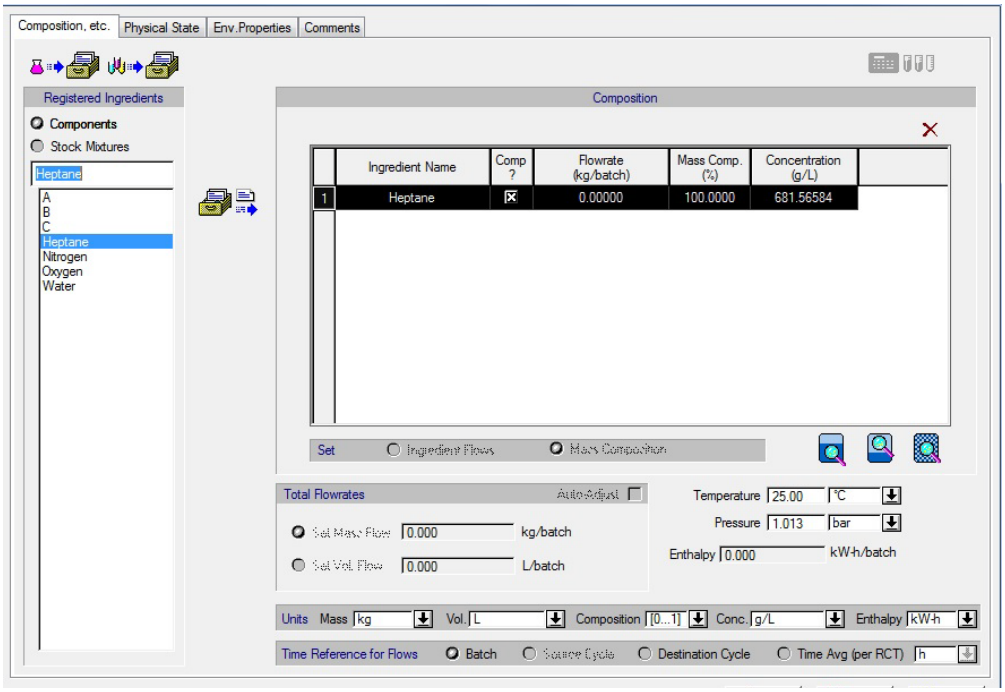


Figure 2.15: The simulation data dialog for the ‘Heptane’ stream.

Please note the following with respect to the simulation data dialog of streams:

1. You can charge multiple components in the same stream if you wish. To do this, simply add additional component names from the ‘Registered Ingredients’ listing. If the ‘Ingredient Flows’ option is selected, you can specify the corresponding amounts of added ingredients. The computer will automatically calculate the mass (%) and concentration (g/L or mole/L) of each ingredient, the stream’s density (if it is not set by the user), the volumetric flowrate and the activity of the stream. If the ‘Mass Composition’ option is selected, you can specify the total mass or volume flow and the mass (%) of each component. You may also select units for entry and display.
2. In addition to pure components, stock mixtures can be fed (or “charged”) into a process step using an input stream. To add a stock mixture to the stream, select the ‘Stock Mixtures’ option for registered ingredients and follow the same guidelines as for adding components.
3. The pure components (or stock mixtures) that are shown in the list on the left hand side of this dialog are the ones that were added to the project through the Pure Component (or Stock Mixture) registration dialogs (see section 2.1e Registering Components and Mixtures). If there are additional pure components or stock mixtures that are required for this stream, they may be added to the project by clicking the **Register Pure Components** ( ) or **Register Stock Mixtures** ( ) buttons in the upper left corner of the dialog. Once the additional components are added to the project, they may be selected and added to the stream.

4. As an alternative to going through the simulation data dialogs of operations to edit stream properties, you can initialize and edit input streams directly from the flowsheet itself. To do this, double-click on a stream (or right-click on a stream and click **Simulation Data** from the context menu of that stream). This will bring up the same dialog box as the one shown in Figure 2.15. Note that only the feed (input) streams of the flowsheet need to be specified. The flowrates and compositions of intermediate and output streams are calculated by the program. However, the user can specify the physical state properties of these streams.
5. For biotech processes, the extracellular percentage ('Extra-Cell %') of an ingredient represents the fraction of that ingredient in the bulk solution (as opposed to inside the cell). Note that for the Extra-Cell % column to appear in a stream's simulation data dialog, a specific Primary Biomass component must first be chosen within the pure component registration dialog (see Figure 2.3). For more information on this topic, please refer to the β-Galactosidase example (see section 2.3 The b-Galactosidase Process).
6. If the plant operation mode is batch, all flowrates are reported on a per-batch basis (or per cycle of source or destination process step). If the process plant is set to operate in continuous mode, then all flowrates are reported on a per-hour basis. The choice for mass units can be made from each stream's dialog. This choice overwrites the default choices of physical units for the whole process as specified by selecting **Process Options ▸ Physical Units Options** on the **Edit** menu.
7. The 'Environmental Properties' tab of a stream's simulation data dialog displays the concentrations and daily throughputs of the environmental and aqueous properties of the stream (TOC, CaCO3, TP, TKN, COD, ThOD, BOD5, BODu, etc). All values are for display only and cannot be edited by the user through this dialog box. However, the environmental properties of the pure components contained in that stream (which contribute to the above stream properties) can be edited by selecting **Pure Components ▸ Register, Edit/View Properties** on the **Tasks** menu. To edit the environmental properties of a pure component, double-click on the desired component in the list of registered pure components and in the dialog that comes up click the 'Aqueous' tab.

For more details on streams and their properties, see Chapter 4 (Streams).

After you have specified the composition of the 'Heptane' stream, click **OK** to return to the operating conditions tab for the 'Charge Solvent' operation. Then, specify the amount of material that is going to be charged (1200 L). Notice that there are several ways that the duration of this operation can be specified. For this example, change the setup time of your charge to 5 minutes and set the volumetric flowrate to 30 L/min so that your tab looks like the one shown in Figure 2.14.

To enter a new value in different units than the ones selected you must first change the units prior to entering the new value.This is necessary since the units selection list acts as a unit converter, and changing the units will automatically convert the existing value to the selected units.

Please also visit the 'Volumes', 'Vent/Emissions', 'Labor etc', and 'Scheduling' tabs to see what they contain. A brief description of each of these tabs follows:

- 'Volumes' tab: Through this tab, the user can specify the maximum and minimum allowable working / vessel volume for this operation (i.e., by the end of the charge operation the vessel should not be more than 90 % full). In 'Design Mode' this is taken into

account for sizing the equipment. In 'Rating Mode', the program makes sure that a vessel is not overfilled or the level does not drop below the agitator level.

- 'Vent/Emissions' tab: Through this tab, the user can specify which volatile organic compounds (VOCs) will be emitted, whether a sweep gas will be used (for emissions associated with reaction and crystallization operations), and what temperature the vent condenser should be set at. SuperPro Designer is equipped with VOC emission models that are accepted by EPA. For more details, see Chapter 10 (Emissions).
- 'Labor, etc.' tab: Through this tab, the user can specify labor requirements and auxiliary utilities.
- 'Scheduling' tab: The is the right-most tab of all batch unit procedures. Through this tab, the user can specify the start time and duration for an operation. Note that no scheduling information is required for unit procedures that are operated in continuous mode.

Depending on the complexity of an operation, additional tabs may be used to display other pertinent variables.

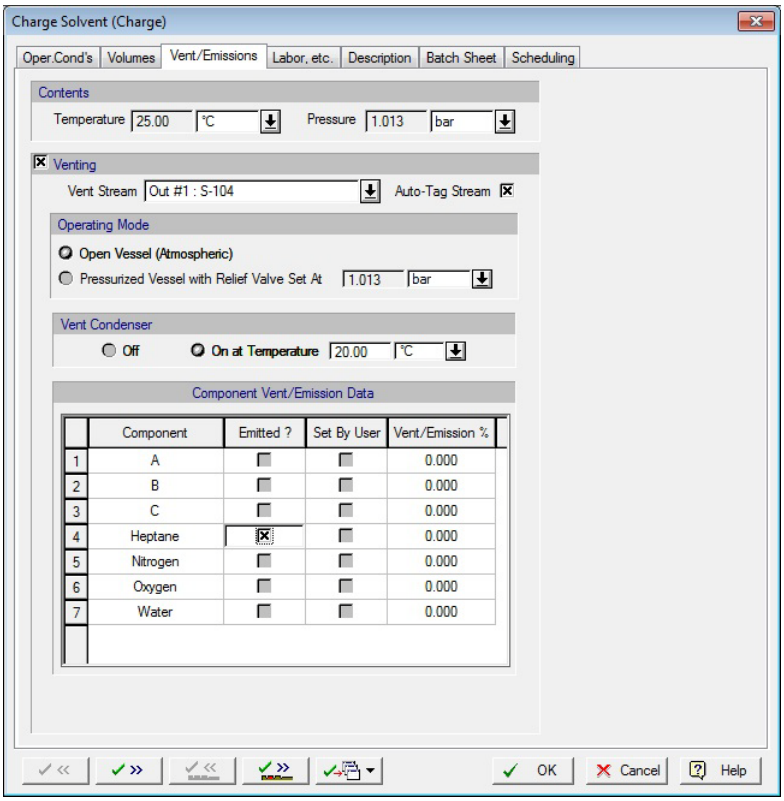


Figure 2.16: The 'Vent/Emissions' tab for the first Charge operation ('Charge Solvent') in procedure 'P-1'.

For the heptane charge in your example process ('Charge Solvent'), please switch to the 'Vent/Emissions' tab and click the 'Venting' box (see Figure 2.16). By default, the port that is connected to stream 'S-104' is selected as the venting port.

Next, turn on the Vent Condenser at 20 degrees C. Then check the 'Emitted ?' box next to the 'Heptane' component. After the simulation, please remember to visit the simulation data dialog of stream 'S-104' and check the amount of emitted 'Heptane'. Note that for particulates and other components for which emission models are not available, the user can directly specify the emission percentage. For this operation, leave all the default values for the 'Volumes', 'Labor, etc.' and 'Scheduling' tabs.

Next, click **OK, Next Operation** (✓») on the simulation data dialog to move to the second Charge operation (named 'Charge Reactant A') in this unit procedure. For this operation, use stream 'S-102' to add 50 kg of material 'A' to the reactor (remember to visit the stream's simulation data dialog and add material 'A' to the stream). Also, specify a 5 minute setup time, select the 'Set by User' process time option and set the process time equal to 20 minutes (see Figure 2.17). Keep the default values for the other tabs.

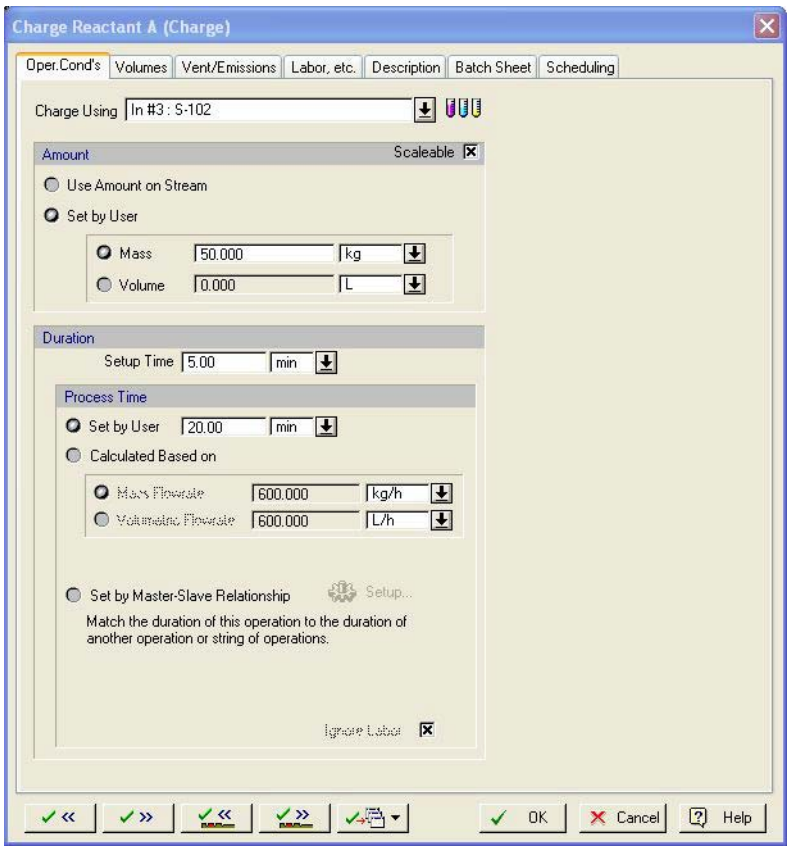


Figure 2.17: The 'Oper. Cond's' tab for the 2nd Charge operation ('Charge Reactant A') in procedure 'P-1'.

Then, click **OK, Next Operation** again to move to the final Charge operation (named 'Charge Reactant B'). For this operation, use stream 'S-103' to add 40 kg of material 'B'. Also, change the setup time to 5 minutes, select the 'Set by User' process time option and set the

process time equal to 30 minutes (see Figure 2.18). Again, keep the default values for the other tabs.

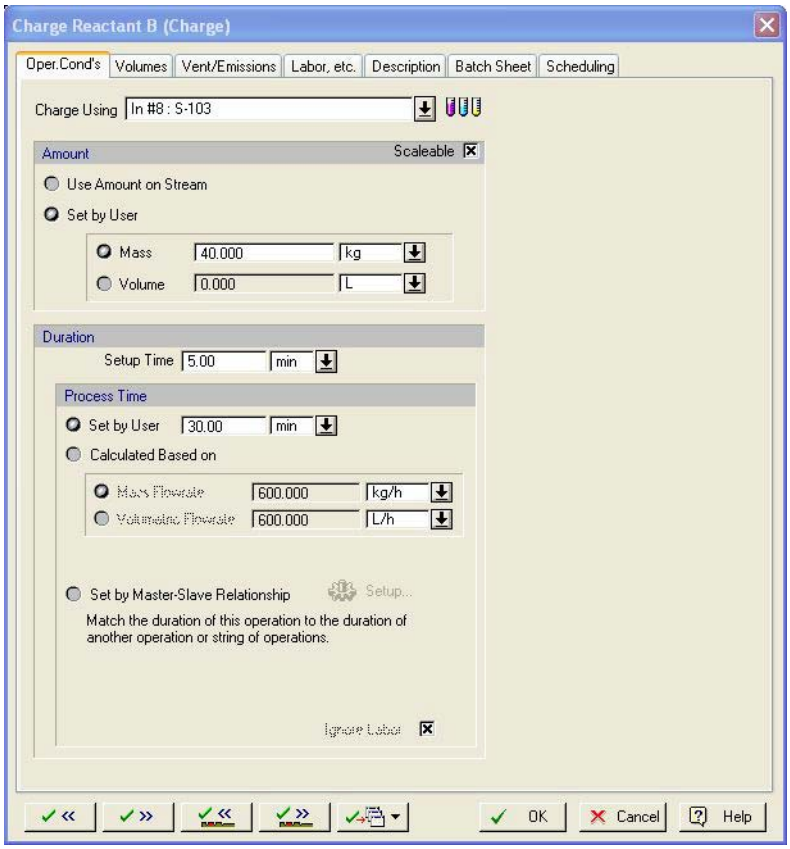


Figure 2.18: The 'Oper. Cond's' tab for the 3rd Charge operation ('Charge Reactant B') in procedure 'P-1'.

Click **OK, Next Operation** once more to move to the Batch Stoichiometric Reaction operation (named 'React'). Notice that the 'Oper. Cond's' tab is different for this operation than it was for the charge operations. Also, two additional tabs are present. These include a 'Fed Batch' tab that contains specification options for fed-batch supply of reactants, and a 'Reactions' tab where the reaction parameters will be specified. From the operating conditions tab, ensure the final temperature is specified as 25°C and set the reaction time equal to 6 hours. If 'Chilled Water' is not already specified as the heat transfer agent, select it by clicking the 'Agent' drop-down list box and double-clicking on 'Chilled Water' in the 'Heat Transfer

Agents' drop-down listing that pops up (see Figure 2.19). Keep the default values of all other parameters in this tab.

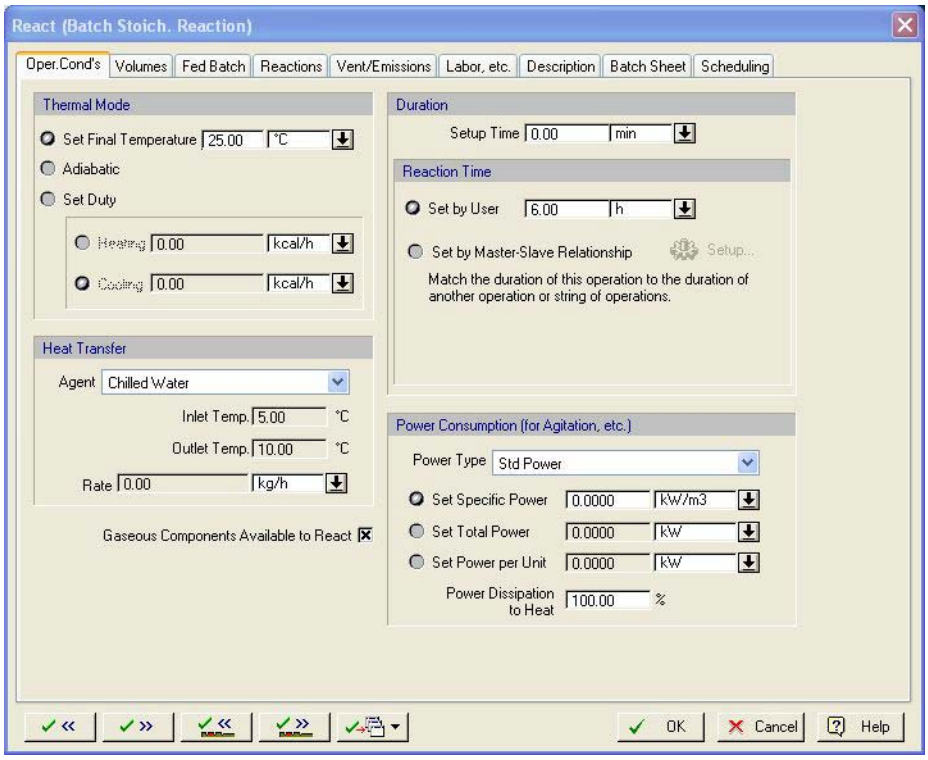


Figure 2.19: The 'Oper. Cond's' tab for the Batch Stoichiometric Reaction operation in procedure 'P-1'.

Next, moving to the 'Volumes' tab, notice that you can specify a maximum and minimum working-to-vessel volume ratio. Verify that the 'Max Allowable Working/Vessel Volume' is set to 90%. Then move to the reactions tab (see Figure 2.20).

In this tab, you will need to specify the parameters describing a reaction in which a molecule of reagent (A) combines with a molecule of reagent (B) to form a molecule of product (C):

$$A + B \rightarrow C$$

To enter this, click **Edit Stoichiometry** ( ) to bring up the 'Stoichiometry Balance' dialog for Reaction #1 (see Figure 2.21). Introduce the reactants (pure components 'A' and 'B') and the product (pure component 'C') using the **Add a Reactant** and **Add a Product** toolbar buttons (, located above the reactant and product tables, respectively). Select the 'Molar' option for the specification of the stoichiometric coefficients and keep the default unit molar coefficient for everything; for more details on specifying the stoichiometry balance for a

reaction, see 2.2d Initialization of Reaction Operations. Now, click **OK** to close this dialog and return to the 'Reactions' tab.

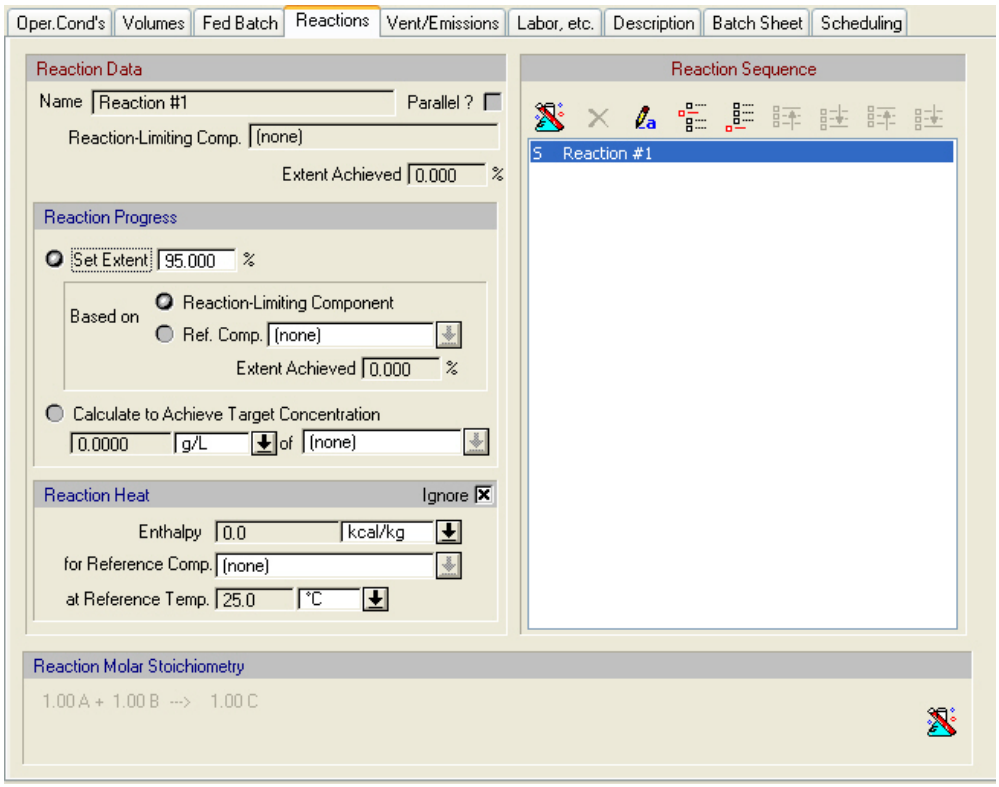


Figure 2.20: The 'Reactions' tab for Batch Stoichiometric Reaction operation 'React' in procedure 'P-1'.

In addition to specifying the stoichiometric reaction coefficients, you will need to specify the extent of the reaction. For this example, set the extent to 95%, as was done in Figure 2.20.

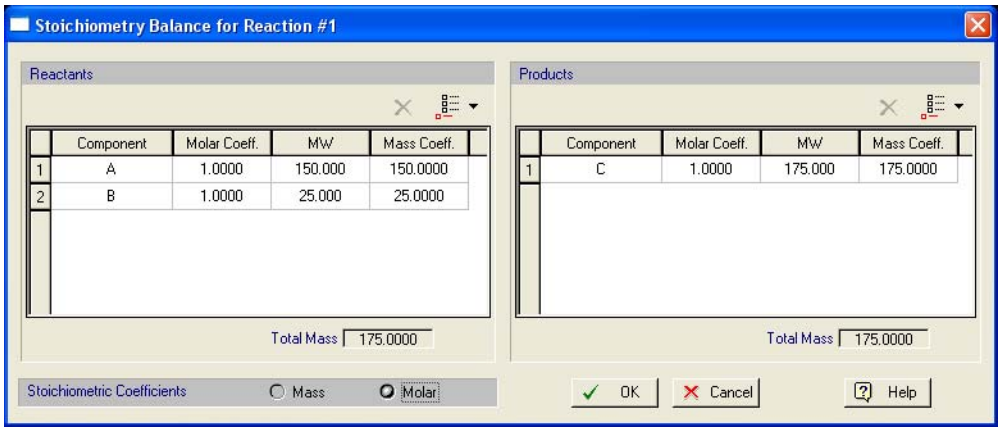


Figure 2.21: The 'Stoichiometry Balance' dialog box for the reaction of the example.

Leave all the default values for the 'Vent/Emissions', 'Labor. etc.', and 'Scheduling' tabs and click **OK, Next Operation** to move to the 'Operation Data' dialog for the Transfer Out operation ('Transfer to PFF-101'). In the operating conditions tab (see Figure 2.22), use the drop-down menu at the top of the screen to specify which stream will be used for the transfer operation (stream 'S-105' is the only choice for this example). In addition, in order to accurately capture the time required for this operation, set the duration to be the same as the duration of the filtration operation in procedure 'P-2'. To do that, select the 'Set By Master-Slave Relationship' duration option and then click the **Setup** button. Through the dialog that comes up, select 'P2 (in PFF-101)' as the Master Procedure (through the 'Another Procedure' drop-down list) and 'FILTER-1 (Cloth Filtration)' as the Master Operation (through the 'Match a Single Operation' drop-down list). This will ensure the reactor will be considered "utilized" during the entire cloth filtration operation, since the reactor will not be completely emptied until the filtration is complete. In addition, make sure the "Ignore Labor" checkbox at the bottom of this dialog is checked on. This will ensure labor required to transfer the materials between the reactor and the filter will not be double-counted; instead the labor required for the transfer will be accounted for within the cloth filtration operation in unit procedure 'P-2'. You can leave the default values for the other tabs in this dialog. Please click **OK** to return to the flowsheet.

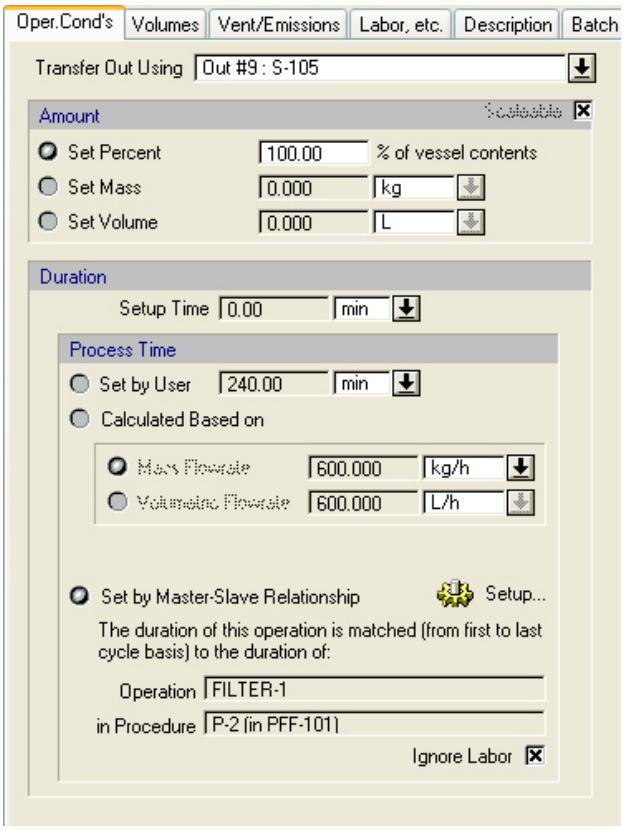


Figure 2.22: The 'Oper. Cond's' tab for Transfer Out operation 'Transfer to PFF-101'in procedure 'P-1'.

Plate and Frame Filtration Procedure

Next, you will need to initialize the operations in the filtration procedure ('P-2'). Please right-click on unit procedure 'P-2' and select **Operation Data ▸ FILTER-1 (Cloth Filtration)** from the context menu of that unit procedure. This will bring up the 'Operation Data' dialog for the Cloth Filtration operation (named 'FILTER-1').

The operating conditions tab for this operation is shown in Figure 2.23. For the purposes of this example, let us assume that reagents 'A' and 'B' are completely soluble in 'Heptane', whereas the product 'C' is virtually insoluble in 'Heptane'. In the 'Particulate Component Removal' table that is available on the top left corner of this tab, please specify that 95% of your product 'C' will be removed from the feed stream and will remain on your filter, whereas the rest will end up in the filtrate.

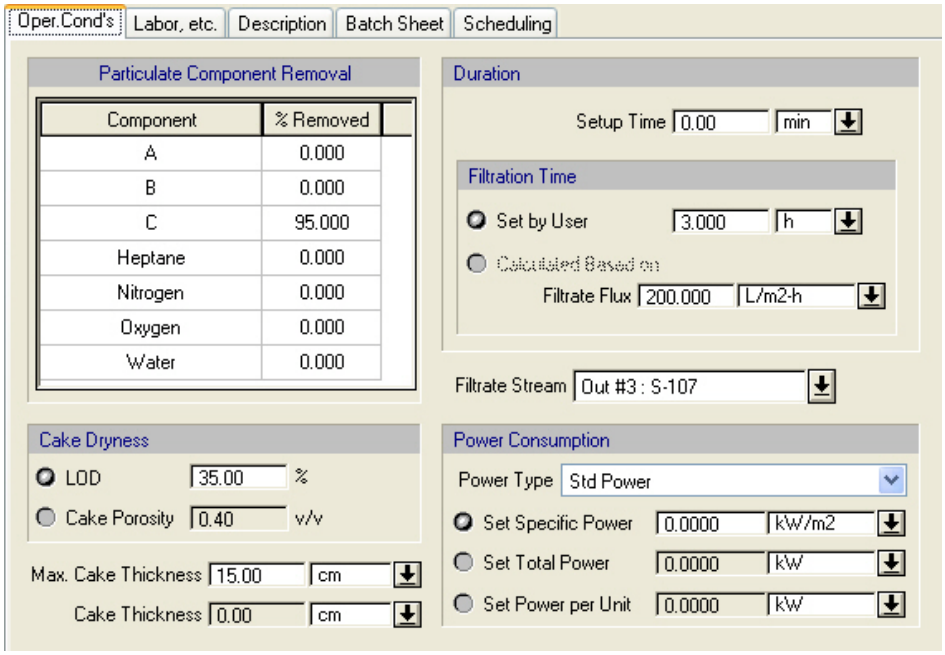


Figure 2.23: The 'Oper. Cond's' tab for Cloth Filtration operation 'FILTER-1'in procedure 'P-2

Also notice that you can specify a cake dryness either based on loss on drying (LOD) or cake porosity. This value will cause a portion of the 'Heptane' solvent and of soluble components 'A' and 'B' to be held in your wet cake. Please change the LOD for your filtration to 35%. By specifying a LOD of 35%, you are telling the program that only 65% of wet cake is the insoluble product C. For this operation, please specify a filtration time of 3 hours. Keep the rest

of the parameters (such as the filtrate flux of 200 L/m^2-h) as they are, and keep stream ‘S-107’ as the filtrate stream.

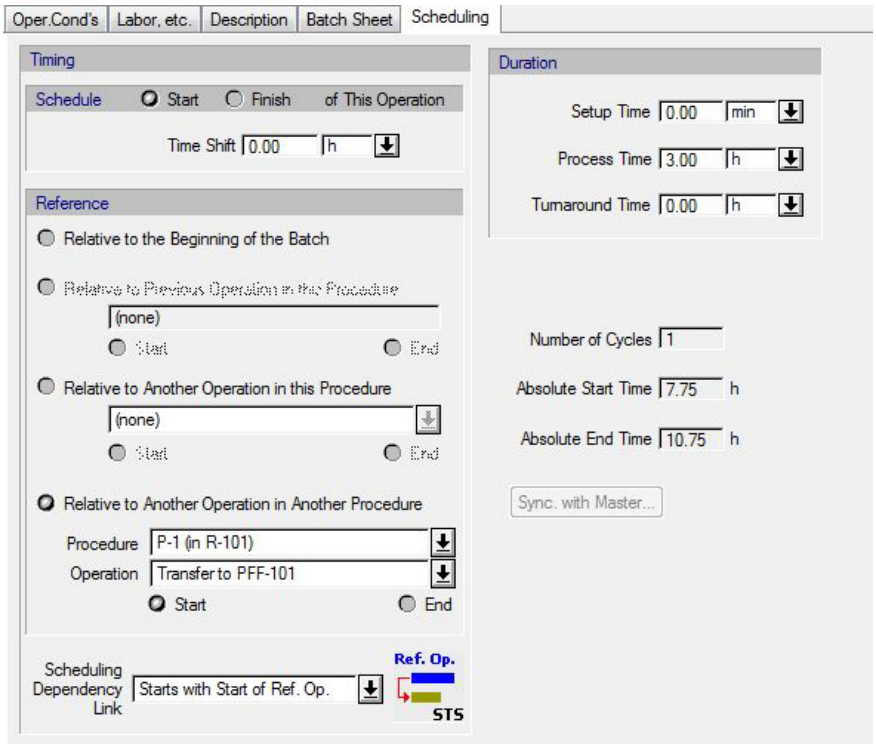


Figure 2.24: The ‘Scheduling’ tab for Cloth Filtration operation ‘FILTER-1’in procedure ‘P-2’.

Next, please visit the ‘Scheduling’ tab of the filtration operation. This tab is common to all operations in batch unit procedures. By default, the first operation in any batch unit procedure is scheduled to start relative to the beginning of the batch. In order to accurately schedule your filtration, you will need to change the start time to be relative to the start of the Transfer Out operation ‘Transfer to PFF-101’ in procedure ‘P-1’ (see Figure 2.24). The Scheduling Dependency Link selection will be automatically updated to reflect the changes.

Next, click **OK, Next Operation** to move to the ‘Operation Data’ dialog for Cake Wash operation ‘CAKE-WASH-1’. In the ‘Cake Wash’ tab (see Figure 2.25), you will need to specify which stream will provide the wash solvent and which one will remove the waste. For this example, keep stream ‘S-109’ as the wash-in stream and select stream ‘S-108’ as the wash-out stream. In addition, you will need to specify what solvent will be used for the wash. To do this, click **View/Edit Stream Composition and/or Amount** ( ) to open the simulation data

dialog for the wash-in stream. Add pure component 'Heptane' to the stream and click **OK** to return to the operating conditions tab.

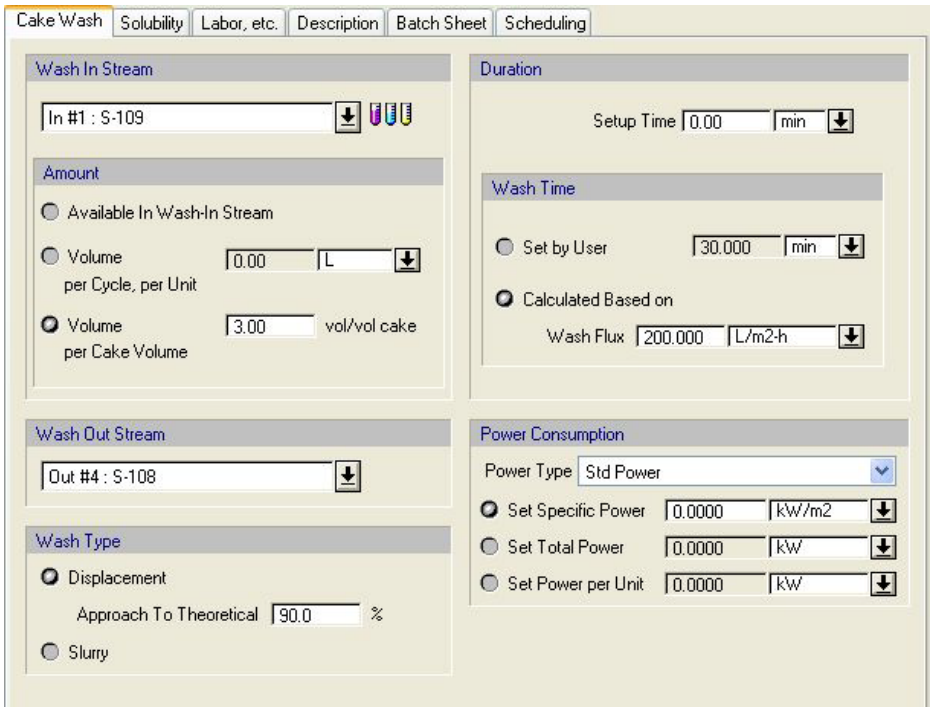


Figure 2.25: The 'Cake Wash' tab for Cake Wash operation 'CAKE-WASH-1' in procedure 'P-2'.

Notice that you can choose among three specification options for the volume of wash to use:

- Available In Wash-In Stream,
- Volume per Cycle, per Unit, or
- Volume per Cake Volume.

If the first option is selected, SuperPro Designer will use the amount that is available in the wash-in stream as the wash amount. Therefore, the user must specify the mass or volume of the wash-in stream through the stream's simulation data dialog. Alternatively, you can select the second option and specify the volume of wash to use per procedure cycle and per equipment unit directly, or select the third option and specify the specific volume of wash with respect to the cake volume. For this example, please keep the third option with 3 wash-in stream volumes per volume of cake (which is the default option). Also, set the wash time to be calculated based on a Wash Flux of 200 L/m^2-h and keep the default option for the Wash Type (i.e., Displacement Type with a 90% Approach to Theoretical). Notice that a "slurry" wash will essentially dilute the soluble components trapped in the cake and remove most of them in the

wash stream, whereas a "displacement" wash will remove the soluble components from the cake in a plug-flow fashion.

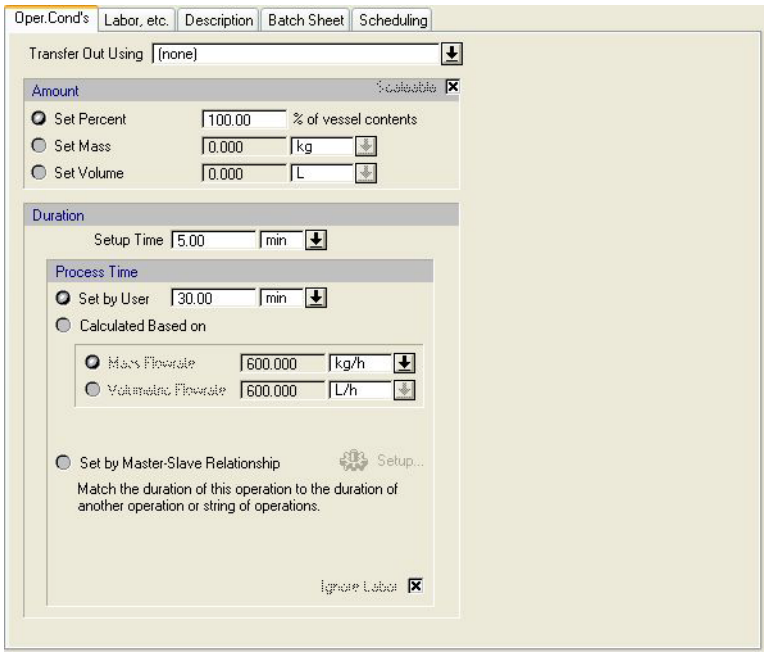


Figure 2.26: The 'Oper. Cond's' tab for the Transfer Out operation n procedure 'P-2'.

Finally, click **OK, Next Operation** to initialize the Transfer Out operation (named 'TRANSFER-OUT-1') in this unit procedure. In this operation, you will need to specify that you are going to transfer out the cake using a specific stream (the 'Cake' stream is the only choice in this case). Furthermore, set a Setup Time of 5 minutes and a (user defined) Process time equal to 30 minutes as illustrated in Figure 2.26. Then, click **OK** to return to the flowsheet.

You have now finished initializing the operations and streams for this example process. Click **Save** on the **File** menu to save your work.

The Process Explorer pane provides a quick and easy way to view and edit all the key resources that have been assigned to a process (e.g., materials, equipment, labor, etc.). To view this pane, click the Process Explorer button ( ) on the main toolbar. Also note that any comments that have been entered for the overall process, its procedures, its streams, or its resources are displayed on the Doc tab of the Process Explorer. This allows the flowsheet to act as a knowledge repository for the process. Please see chapter 8.10 Process Explorer for more information on this topic.

2.1i Simulating the Process and Viewing the Simulation Results

SOLVING MASS AND ENERGY BALANCES

At this point, you can click **Solve M&E Balances** on the **Tasks** menu to perform the simulation. This will cause the program to perform the mass and energy balances for the entire process, estimate the sizes of all pieces of equipment that are in 'Design Mode', and model the

scheduling of each piece of equipment. As a shortcut for performing simulations, you may hit **Ctrl+3** or **F9**, or simply click the **Solve ME Balances** button () on the **Main** toolbar.

VIEWING SIMULATION RESULTS

The following simulation results can then be viewed for this example:

Stream Data

The calculated flowrates and compositions of intermediate and output streams can be viewed by revisiting the corresponding simulation data dialog windows (double-click on any stream line to see its simulation data dialog).

Procedure Data

The procedure start time, end time, and cycle time (its duration), as well as throughput analysis results for a procedure, can be viewed by visiting the corresponding 'Procedure Data' dialog (right-click on the desired unit procedure icon and click **Procedure Data** on the context menu of that procedure).

Operation Data

The calculated parameters for an operation can be viewed by visiting the corresponding 'Operation Data' dialog (right-click on the desired unit procedure icon and choose the operation you are interested in from the **Operation Data** context menu). For instance, you can see how long the Charge Solvent operation takes (recall that its duration was based on a given volume to be charged and a flowrate).

Equipment Contents

The contents of a piece of equipment as a function of time can be viewed by right-clicking on a unit procedure and selecting **Equipment Contents** or **Procedure Activity Overview** on the context menu of that procedure.

Streams & Material Balance Report (SR)

A report containing information on raw material requirements, stream compositions and flow rates, as well as an overall material balance, can be generated and displayed by clicking **Streams & Mat. Balance (SR)** on the **Reports** menu. This report includes an overview of the process, a listing of the raw material requirements, a listing of the compositions of each stream, and an overall component balance. Please generate and view this report now. To see more comprehensive stream reports, please refer to the synthetic pharmaceutical example (see 2.2e Process Analysis), the β-Galactosidase example (see 2.3e Process Analysis) and the industrial wastewater treatment example (see 2.4b Process Analysis). If you wish to customize the stream report, click **Options** on the **Reports** menu and switch to the 'Stream' tab. For more details on reports, see Chapter 12 (Reports).

Equipment Data.

To see the calculated number and size of equipment units, right-click on a unit procedure icon and click **Equipment Data** on the context menu of that procedure. This will bring up the 'Equipment' Data dialog of the equipment resource that hosts that procedure. At this point,

please open the 'Equipment Data' dialog for Plate & Frame Filter 'PFF-101' (shown in Figure 2.27).

Figure 2.27: The Equipment tab for Plate & Frame Filter 'PFF-1'.

All unit procedures have two options for equipment sizing:

- Calculated (Design Mode), and
- Set by User (Rating Mode).

These options can be specified through the 'Equipment' tab of the corresponding 'Equipment Data' dialog. By default, all equipment resources start in 'Design Mode'. In this mode, SuperPro Designer will determine the required number and size of equipment units based on operating conditions and performance requirements.

Usually, there are physical limitations on the available size of processing equipment. For example, a Plate & Frame Filter may not be available with a cloth area greater than 80 m^2. When you are in 'Design Mode', you must specify the maximum available size for the equipment involved (e.g., the 'Max. Filter Area' for the Plate & Frame Filter). If the calculated equipment size exceeds the maximum allowable size, SuperPro Designer will employ multiple pieces of equipment (sized equally) with sizes that do not violate the maximum available size. For your example process, a filter size of roughly 2 m^2 should have been calculated, as shown in Figure 2.27 (this same process model, titled 'GettingStarted9_0a', is also available in subdirectory 'Examples\Misc'). This filter size was calculated from the volume of material that was processed per cycle, the filtrate flux, and the filtration time.

If you change the equipment sizing method to 'Rating Mode', you can specify the size and number of units. SuperPro Designer will then take this information into account in the simulation calculations (equipment size and number of units may affect the material and energy balances, the process time, etc.). Switching to 'Rating Mode' may also affect the interface of some operations of that procedure. To experience this, please select 'Rating Mode' for Plate & Frame Filter 'PFF-101', change the size of the filter to 4 m^2 and click **OK** to return to the flowsheet. Then, revisit the dialog of the filtration operation. In this case, you need to specify either the filtration time or the average filtration flux (remember that in 'Design Mode' you must specify both). Please set the filtrate flux to 150 L/m^2-h and redo the mass & energy

balance calculations by either selecting **Solve M&E Balances** on the **Tasks** menu or clicking **Solve ME Balances** ( ) on the **Main** toolbar. The new results for the filtration operation are shown in Figure 2.28. In general, most batch operations have the capability of calculating their cycle time when the equipment size is specified ('Rating Mode').

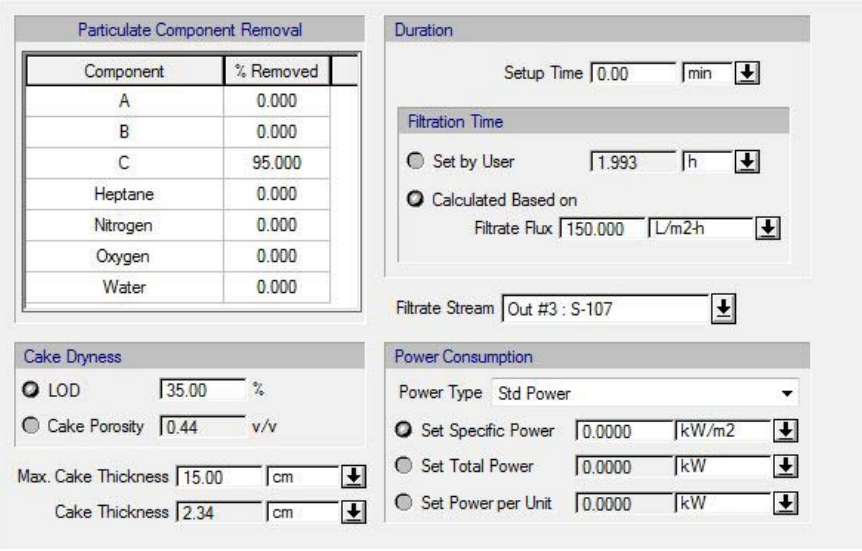


Figure 2.28: The 'Oper. Cond's' tab for Cloth Filtration operation 'FILTER-1' in procedure 'P-2' with the equipment in 'Rating Mode'.

Through the 'Equipment' tab of the 'Equipment Data' dialog, you can also select the specific piece of equipment that is going to carry out the processing step. By default, it is assumed that each unit procedure is carried out in its own (exclusive) equipment. However, two or more different unit procedures can share equipment if they are in batch operating mode and the entire process is also in batch mode. For more information on equipment sharing, see 6.1b Equipment Selection & Sharing and the following two detailed examples: 2.2 The Synthetic Pharmaceutical Process and 2.3 The b-Galactosidase Process.

At this point you have completed the basic initialization steps for the streams, operations, and equipment. As you become more familiar with SuperPro Designer, it will take much less time to do these activities. For instance, all the steps that we have done thus far in this section could be performed in about 15 minutes if you were already familiar with how to use SuperPro Designer

.

Important note about building and initializing large process flowsheets *– when you attempt to simulate complex processes, keep in mind that you don't have to add all the unit procedures at once. You can always add or remove procedures as desired at a later stage. For complex processes, it is highly recommended that you begin your simulation with just a handful (core) unit procedures and add more only after you have successfully completed the simulation for the first phase (streams and operations have been initialized correctly and your mass balances make sense).* ***Similarly, when you are learning how to use SuperPro Designer, the best practice is to build the flowsheet one or two unit procedures at a time, simulating the file and checking the key stream results after each procedure (or set of procedures) has been added.*** *Otherwise mistakes in specifications early in the process may propagate to the rest of the flowsheet and result in large numbers of error and warning messages.*

Before continuing with this tutorial, please change the filtration time back to 3 hours for the **FILTER-1 (Cloth Filtration)** operation within procedure **P-2** by revisiting the **Oper Conds.** tab for that operation.

USING BREAKPOINTS

When simulating large processes it is sometimes useful to solve only part of the process. Setting breakpoints tells the simulator to halt calculations at a certain point. A brief description of this facility is given below.

You can place a breakpoint, and force the M&E balance execution sequence to pause either right before, or right after the solution of a unit procedure. You may even place a breakpoint inside the unit procedure's solution sequence of unit operations.

▶ To Place a Breakpoint on a Unit Procedure...

1. Right click on a unit procedure to bring up its context menu and select **Set Breakpoints**. Through the 'Breakpoints' dialog that appears, you can specify where to break the simulation of the selected unit procedure.
2. Check the place(s) where you wish the simulation to pause and exit this dialog. Notice that red signs ( ) are shown above the procedure's icon to indicate that one or more breakpoints are set on this procedure. The position of the sign indicates whether the break is on the entry (left sign), operations (middle sign) or exit (right sign) of the procedure.

Once a breakpoint is set, next time the 'Solve M&E Balances' command is issued, the simulation calculation sequence will pause at that location. When the simulation sequence is paused, some buttons of the 'Solve' toolbar become active. Also notice that while the simulation has been paused, all unit procedure display another icon underneath that indicates the simulation state of each procedure at that time (as the simulation is paused). The following sequence of images indicate the state of the unit procedure that is *currently being solved*:

Image	Explanation
	A break on entry has been encountered.
	A break on operation has been encountered.
	A break on exit has been encountered.
	A break on entry has been encountered (shown when there are operations that can auto-adjust the flow of process input streams).

Image	Explanation
	A break on material pull-in has been encountered (for operations that can auto-adjust the flow of process input streams).
	A break on operation has been encountered (shown when there are operations that can auto-adjust the flow of process input streams).
	A break on material pull-out has been encountered (for operations that can auto-adjust the flow of process output streams).
	A break on exit has been encountered (shown when there are operations that can auto-adjust the flow of process input streams).

The following sequence of images indicate the state of *all other unit procedures* while the simulation is paused:

Image	Explanation
	The procedure has not been visited yet.
	The procedure has been successfully simulated already.
	The procedure's M&E balances are being solved recursively (as part of loop convergence).
	The solution of the procedure's M&E balances ended unsuccessfully (as part of an un-converged loop).
	The solution of the procedure's M&E balances ended unsuccessfully (an error was encountered)

Notes

1. You can toggle the visibility of the breakpoint icons (above the unit procedure) and of the state icons (below the unit procedure) using the **Show / Hide Breakpoints** ( ) and **Show / Hide Status** () buttons, respectively, on **the Simulation Control** toolbar.
2. To temporarily deactivate breakpoints (without removing them), simply visit the 'Breakpoints' dialog of a unit procedure and click once more on the checked breakpoint location. Notice that the checkmark is now gone but the box has a different shading compared to the other boxes which had not been checked. In addition, after clicking **OK** to confirm the change, the breakpoint sign above the unit procedure icon looks faded (greyed out).
3. When the 'Solve M&E Balances' sequence is paused, you may visit the simulation data dialog of any stream, unit procedure, equipment, or operation, to inspect or even modify values of operating conditions. If you modify the values of streams and/or operations belonging to unit procedures that have already been solved (i.e., the check mark icon appears underneath) or if you modify specifications related to already-solved operations within the unit procedure that is currently being solved, then the new values will not be taken into account until the next 'Solve M&E Balances' command is issued.

CONVERGENCE OF RECYCLE LOOPS

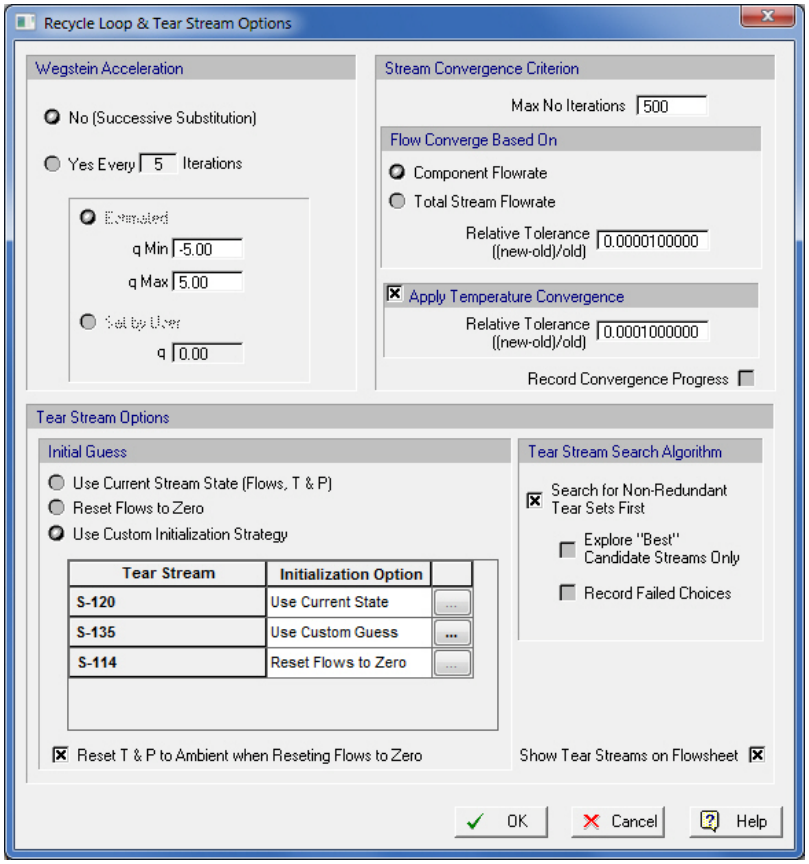


Figure 2.29: Adjusting the convergence parameters in a process that includes recycle loops.

The material of this is only relevant to process flowsheets that include recycle loops. To see an example of a recycle loop, please open file Bgal9_0b, which can be found in the Examples \ Bgal directory of SuperPro Designer. In this file, streams ‘S-102’ and ‘S-108’ are part of a recycle loop. For a description of this file, see 2.3 The b-Galactosidase Process.

SuperPro Designer’s default convergence parameters for flowsheets that include loops (which result in iterative calculations) have been tuned in order to be adequate for most situations. However, occasionally (especially in cases involving highly non-linear models) they may fail to converge. In these cases, you may fine-tune the convergence characteristics for a particular application. To change the convergence parameters for the process with loops, click **Process Options ▸ Recycle Loop & Tear Stream Options** on the **Edit** menu. Alternatively, right-click on an open area of the flowsheet and click **Recycle Loop & Tear Stream Options** on the flowsheet’s context menu.This will bring up the ‘Recycle Loop and Tear Stream Options’ dialog of Figure 2.29.

Below is a list of actions that you can take to improve the system’s performance in converging iterative calculations:

1. Adjust the convergence tolerance ('Relative Tolerance') for stream total or component mass flow and, optionally, temperature. The convergence tolerance is defined as (new value - old value) / old value. Setting the relative tolerance to a larger value may speed up the convergence (but may lead to less accurate simulation results).
2. Switch from convergence based on the total flow to convergence based on individual component flows. This may slow down the convergence process but it will yield more accurate simulation results. This is especially important for process files that deal with components that are in trace amounts, but whose accurate balance is of utmost importance (e.g., hazardous and/or toxic chemicals).
3. Increase the maximum number of iterations.
4. Request that tear streams be initialized to zero flow (for all components) before every new simulation. Normally, in cases where the process simulation has been converged once, the initially guessed state for tear streams is their current state at the end of the previous (converged) simulation. In most cases, this leads to a faster convergence the next time the mass and energy balances are solved. However, after a convergence failure, it may be better to start with zero values.
5. Adjust the Wegstein algorithm parameters (q_{min}, q_{max}, and q). If the convergence procedure seems to be unstable, raising the value of q_{min} (i.e., making it less negative) may improve convergence; if it is converging very slowly but monotonically, you might lower q_{min}; and if it is converging in an oscillatory manner, try raising q_{max}. You also have the option of adjusting the value of q. If q is between zero and 1, the procedure is a modified successive substitution; if q is negative then the convergence is accelerated.
6. Switch from Wegstein acceleration to successive substitution. This may slow down the convergence calculations but will increase the likelihood of convergence.
7. Select a different tear stream for a recycle loop by right clicking on a specific stream (that is part of the loop) and selecting 'Preferred Tear'. The current tear streams are identified on the flowsheet (with two red slashes) if you check the 'Show Tear Streams on Flowsheet' option that is available in the 'Recycle Loop and Tear Stream Options' dialog.

2.1j Setting the Process Scheduling Information

The following terms are used for batch process scheduling:

Term	Description
Annual Operating Time (AOT)	The number of hours per year the plant is devoted to making a specific product.
Campaign	An uninterrupted run of batches.
Batch Time	The start to finish time for a single batch.
Cycle Time	The time between two consecutive batch starts. This is sometimes referred to as the recipe or plant cycle time.
Minimum Cycle Time	The minimum possible cycle time based on the time (scheduling) bottleneck.
Cycle Time Slack	The difference between the actual and minimum cycle times.

If the process is in batch mode (as is the case for your example process), you should provide process scheduling information before performing a simulation. SuperPro Designer allows you to specify the following scheduling data:

1. For each operation:
   (a) the process time,
   (b) the setup and turnaround times, and
   (c) the starting time.
2. For each procedure, the number of cycles.
3. For the entire plant:
   (a) the available AOT,
   (b) the number of campaigns per year,
   (c) the number of batches per year, and either:
   (d) the cycle time, or
   (e) the cycle time slack.

Scheduling of operations was explained in Section 2.1h Initializing Unit Procedures. In that section, the 'Scheduling' tab of a filtration operation was shown in Figure 2.24. Through the 'Scheduling' tab, you can specify the start time of an operation relative to the beginning of a batch or relative to the start or end of other operations in the same procedure or in a different procedure. You may also specify the process time (if it is not calculated by the model), the setup time and the turnaround time for an operation.

To specify the number of cycles per batch for a procedure (the same number will apply to all operations of the procedure), simply right-click on the unit procedure's icon and select **Procedure Data** from the corresponding context menu. By default, all procedures start with one cycle.

At this point, please change the sizing mode of the P&F filter PFF-101 to 'Design' by right clicking on the equipment icon and selecting 'Equipment Data' in the context menu that appears. To specify scheduling information for an entire process, click **Recipe Scheduling Information** on the **Tasks** menu. This will bring up the 'Recipe Scheduling Information' dialog shown in Figure 2.30.

For your example process (simulated in 'Design Mode'), please change the number of batches per year to 20. This implies that your example process will be run in a pilot plant 20 times this year (it is assumed that the equipment used by this process is used by other processes the rest of the year). In addition, please change the recipe cycle time for this process to 12 hours to reflect the completion of one batch during every 12-hour shift (and the completion of the whole 20-batch campaign in approximately 240 hours). Click **Update** ( ) to see the actual annual operating time (AOT) that the plant is utilized by this process (see Figure 2.30).

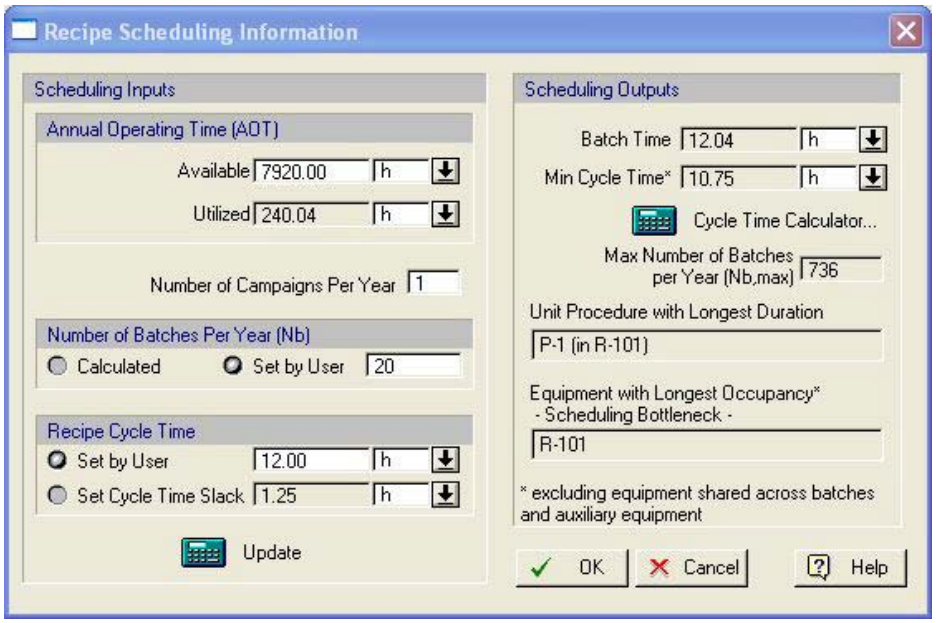


Figure 2.30: Specifying the scheduling information for a batch process.

Based on the scheduling information and the available AOT specified for the plant, the system will do the following:

1. Make sure there is no conflict created by the specified start time and end time of processing steps. Conflicts can be created if the cycle times of procedures that share equipment overlap.
2. Make sure there is no conflict between the specified available AOT, the specified or calculated number of batches, and the specified or calculated recipe cycle time.
3. Calculate the number of batches (if not set by user), the recipe batch time, the recipe cycle time (if not set by user), the recipe cycle time slack (if not set by user), the utilized AOT, the plant's minimum cycle time (with maximum batch overlapping), the maximum number of batches possible, the longest procedure (i.e., the procedure with the longest total cycle time) and the scheduling bottleneck equipment (the equipment with the longest occupancy time).

2.1k Viewing Scheduling, Equipment Utilization and Resource Tracking Results

A variety of scheduling, equipment utilization and resource tracking tools are included in SuperPro Designer. These include:

- Operations / Equipment Gantt Charts,
- Main and Auxiliary (CIP Skids, SIP Panels) Equipment Occupancy Charts,
- Resource Demand Charts, and
- Resource Inventory Charts.

OPERATIONS / EQUIPMENT GANTT CHARTS

The Operations Gantt Chart and the Equipment Gantt Chart display scheduling and equipment utilization information, respectively, for a batch process recipe in the form of a Gantt Chart. These charts can be generated either for a single batch or for multiple batches using dedicated items on the **Charts ▸ Gantt Charts** menu. Note that this menu is only available if the plant operation mode is batch (see 2.1c Specifying the Mode of Operation for the Entire Plant).

Please generate the single-batch Operations Gantt Chart for your example process by selecting **Gantt Charts ▸ Operations GC** on the **Charts** menu. It should look similar to Figure 2.31 below. The left view (spreadsheet view) displays the name, duration, start time and end time for each activity participating in the overall scheduling and execution of the recipe. This can be either an elementary activity or an activity summary. In the Operations Gantt Chart, an elementary activity corresponds to an operation executed during a single procedure cycle. For this example, activity summaries are shown for unit procedures and for the complete recipe. You can expand or collapse activity summaries by clicking on the + or – signs in the boxes to the left of activity names. The right view (chart view) displays a bar for each activity, whose horizontal position and length indicate the start time and duration, respectively, of that activity.

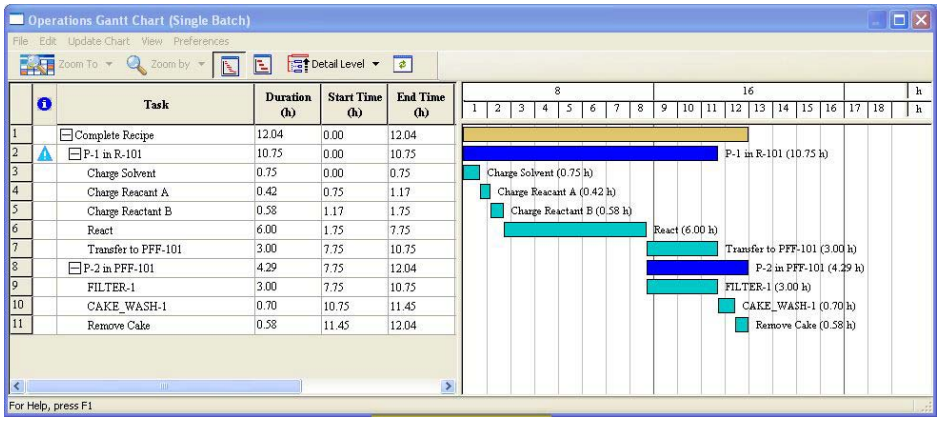

Operations Gantt Chart (Single Batch)
File Edit Update Chart View Preferences
Zoom To
Zoom by
Detail Level
Task
Duration (h)
Start Time (h)
End Time (h)
1 Complete Recipe 12.04 0.00 12.04
2 P-1 in R-101 10.75 0.00 10.75
3 Charge Solvent 0.75 0.00 0.75
4 Charge Reacant A 0.42 0.75 1.17
5 Charge Reactant B 0.58 1.17 1.75
6 React 6.00 1.75 7.75
7 Transfer to PFF-101 3.00 7.75 10.75
8 P-2 in PFF-101 4.29 7.75 12.04
9 FILTER-1 3.00 7.75 10.75
10 CAKE_WASH-1 0.70 10.75 11.45
11 Remove Cake 0.58 11.45 12.04
8
16
h
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18
P-1 in R-101 (10.75 h)
Charge Solvent (0.75 h)
Charge Reacant A (0.42 h)
Charge Reactant B (0.58 h)
React (6.00 h)
Transfer to PFF-101 (3.00 h)
P-2 in PFF-101 (4.29 h)
FILTER-1 (3.00 h)
CAKE_WASH-1 (0.70 h)
Remove Cake (0.58 h)
For Help, press F1

Figure 2.31: The Operations Gantt Chart for a single batch.

The Equipment Gantt Chart interface is similar to that of the Operations Gantt Chart. Please generate the single-batch Equipment Gantt Chart for your example process by clicking **Gantt Charts ▸ Equipment GC** on the **Charts** menu. In this chart, the elementary activity corresponds to the time frame that an equipment unit is kept busy by an operation during a procedure cycle. In this example, activity summaries are shown for unit procedures (corresponding to the time frame that an equipment unit is kept busy by a procedure), for equipment (corresponding to the time frame that an equipment unit is kept busy by all procedures it hosts), and for the complete recipe (named ‘total occupancy time’).

In addition to displaying scheduling information, Gantt Chart interfaces also present you with a graphical way to modify scheduling parameters for an activity and immediately visualize the effects on the entire batch production. In fact, anything you can accomplish with the simulation data dialog interfaces described in 2.1h Initializing Unit Procedures and 2.1j Setting the Process Scheduling Information, you can also accomplish from the Gantt Chart interfaces. To see this, simply double-click on a bar or right-click on a bar and select the uppermost entry on

the context menu for that bar. This will display the simulation data dialog for the corresponding activity. For example:

- if the bar corresponds to an operation, it will display the 'Operation Data' dialog for that operation;
- if the bar corresponds to a unit procedure, it will display the 'Procedure Data' dialog for that unit procedure;
- if the bar corresponds to an equipment resource (available only in Equipment Gantt Charts), it will display the 'Equipment Data' dialog for that piece of equipment;
- if the bar is the one at the top of the chart (named 'complete recipe' in Operation Gantt Charts and 'total occupancy time' in Equipment Gantt Charts), it will display the 'Recipe Scheduling Information' dialog (see Figure 2.30).

If you change the simulation parameters in the above dialogs, you must click **Redo Calc. & Update Chart** ( ) on the toolbar or **Update Chart** on the chart's main menu. This will solve the mass and energy balances again and it will update the Gantt chart to reflect the new scheduling settings for the recipe.

You can change the style (e.g. bar width, time scale, etc.) and contents (e.g., displayed activity summaries) of a Gantt Chart by selecting **Styles** on the **Preferences** menu of the chart. You may also use the items in the **File** menu of the chart to print the chart, export scheduling data to MS-Excel or MS-Project, or export the chart as a Windows Metafile (.wmf). Also note that if you generate an Operations Gantt Chart or an Equipment Gantt Chart for multiple batches, you can change the default number of batches shown on the chart by right-clicking on the chart and selecting **Set Number of Batches** from the chart's context menu.

Please refer to the synthetic pharmaceutical example (see Figure 2.55) and the β-Galactosidase example (see Figure 2.68) to see Gantt Charts for more complex processes. For more information on these charts, see 7.4 The Operations Gantt Chart (OGC) and 7.5 The Equipment Gantt Chart (EGC).

EQUIPMENT OCCUPANCY CHARTS

Another way of visualizing the execution of a batch process as a function of time is through the Equipment Occupancy Chart. This chart provides a graphical representation of the usage and idle times associated with each equipment unit during batch processing. Each chart can be generated either for a single batch or, preferably, for multiple batches using dedicated items on the **Charts ▸ Equipment Occupancy** menu.

Please generate this chart for your example process by selecting **Equipment Occupancy ▸ Multiple Batches** on the **Charts** menu. By default, two batches are shown. To add more, right-click on the chart to bring up the chart's context menu and select **Set Number of Batches**. Please change the number of batches to 3 and press **OK**. Your chart should look similar to the one shown in Figure 2.32.

You can change the scale at the bottom of the Equipment Occupancy chart (and other resource charts) by right-clicking an open area of the chart, selecting **Edit Style**, and clicking the Time Line tab. Then click **Customize** under the **Style Definition** heading in order to specify different major and/or minor units, relative vs. absolute time basis, etc.

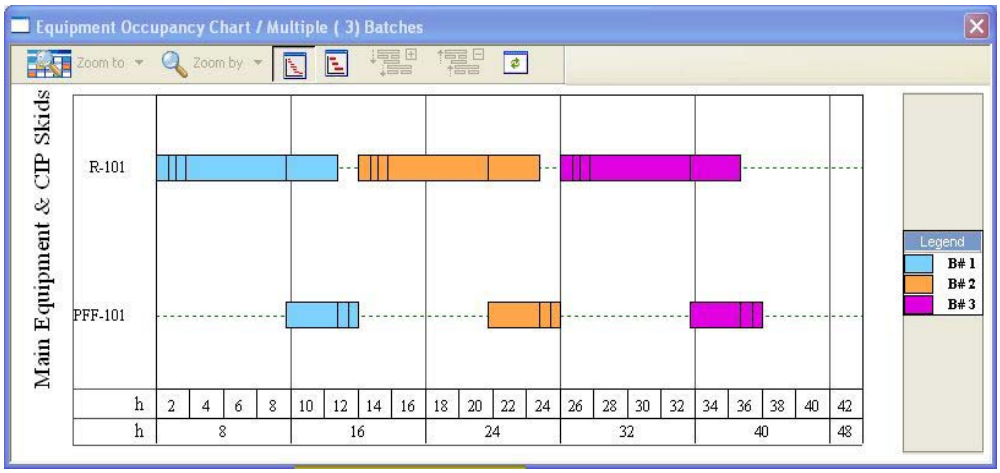


Figure 2.32: The Equipment Occupancy Chart for three consecutive batches.

For each equipment unit, the occupancy time associated with each individual operation is represented by a bar. White space represents idle time. Placing the mouse pointer over a bar will display the name of the operation that corresponds to that bar. Right-clicking on a bar will bring up its context menu. On this menu, you can click **Operation Data** to display the 'Operation Data' dialog for the corresponding operation, or **Procedure Data** to display the 'Procedure Data' dialog for the corresponding unit procedure, or **Equipment Data** to display the 'Equipment Data' dialog for the corresponding equipment. In the 'Scheduling' tab of that dialog, you can see the total equipment occupancy time per batch (as well as additional information).

The equipment with the least idle time between consecutive batches (or, equivalently, the longest occupancy time per batch) is considered the *time (or scheduling) bottleneck* (R-101 in this case). This is the equipment that determines the maximum number of batches per year. Its occupancy time per batch corresponds to the minimum cycle time of the recipe (the minimum possible time between two consecutive batch starts). Based on the scheduling specifications for this example (including the original 3-hour filtration time), the occupancy time per batch for R-1 is 10.75 hours. The total equipment occupancy time per batch (12 hours in this case) corresponds to the actual cycle time of the recipe (the actual time between two consecutive batch starts). To view this information, right-click on an empty area in the chart to bring up the chart's context menu and select **Scheduling Summary**. This will display the 'Recipe Scheduling Summary' dialog for the process. That dialog presents (for display purposes only) the same information as the 'Recipe Scheduling Information' dialog of Figure 2.30. To change the style and contents of the Equipment Occupancy Chart, right-click on an empty area in the chart to bring up the chart's context menu and select **Edit Style**.

Please refer to the synthetic pharmaceutical example (see Figure 2.56) and the β-Galactosidase example (see Figure 2.64) to see Equipment Occupancy Charts for more complex processes. For more information on Equipment Occupancy Charts, see 7.6 The Equipment Occupancy Chart (EOC).

RESOURCE DEMAND CHARTS

In addition to creating Gantt charts for equipment utilization and operations, SuperPro Designer automatically generates graphs of resource demand as a function of time for such things as raw materials, labor, heating and cooling utilities, and power. These can be accessed through the **Charts** menu. For instance, to view the labor demand for this example process, select **Labor ▸ Multiple Batches** on the **Charts** menu. Next, in the labor resource selection dialog that pops-up, keep the default selection ('Operator') and click **OK**. Figure 2.33 displays the 'Operator' labor resource demand graph for two consecutive batches. To add more batches, right-click on the chart to bring up the chart's context menu and select **Set Number of Batches**. As shown in this chart, a two operators are required to handle this process. If you move the cursor close to a peak, SuperPro Designer displays the operations which create that peak.

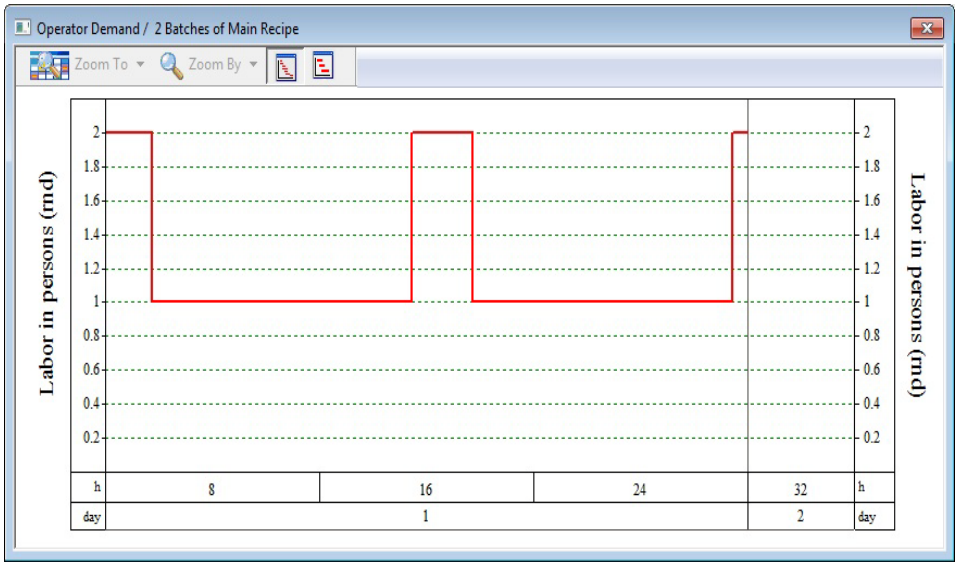


Figure 2.33: The 'Operator' labor resource demand chart for the example process.

To change the contents (variables displayed) and style (e.g., color, thickness, time scale, etc.) of a resource demand graph, right-click on the chart to bring up its context menu and select **Edit Style**. Through context menu commands you can also print a chart, export a chart as a Windows Metafile (.wmf), or export its data into a file in Excel format with a discretization time interval that can be specified by the user. This is a useful feature if you wish to combine demands for a certain resource from multiple process files in Excel.

Please refer to the synthetic pharmaceutical example (see Figure 2.57) and the β-Galactosidase example (see Figure 2.69) to see resource demand charts for more complex processes.

RESOURCE INVENTORY CHARTS

SuperPro Designer can also analyze and display inventory information for material resources. Recall that 50 kg of material 'A' are used in each batch. Suppose that there is a 300kg storage capacity for 'A' and an opening inventory of 100kg. Suppose further that the loading rate of material 'A' into storage is 200 kg/h. How often should shipments of 'A' be scheduled? Please

select **Materials ▸ Entering, Inventory ▸ Multiple Batches** on the **Charts** menu. Select pure component 'A' from the pure components drop-down list box and click the **Supply Info** button. This will bring up the 'Resource Inventory Data' dialog for the selected ingredient. Fill out the dialog as shown in Figure 2.34. This will tell SuperPro Designer that the supply of material 'A' should be replenished when the inventory falls to 10% (or 30 kg) of the capacity. The replenishment should be halted when the inventory reaches 85% (or 255 kg) of storage capacity. Click **OK** to return to the previous dialog.

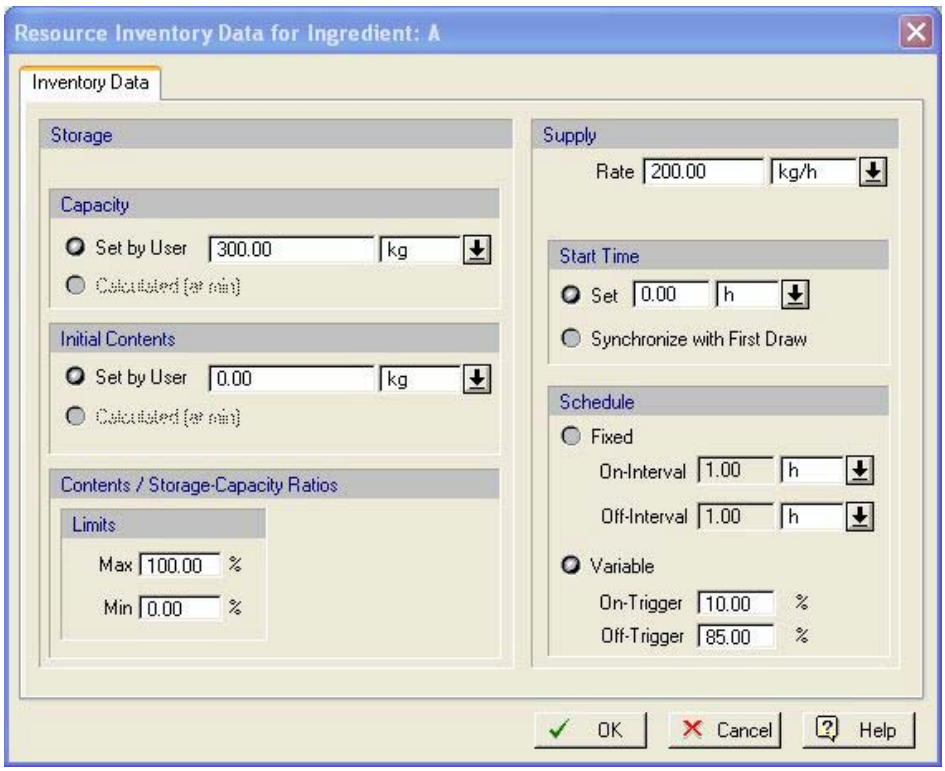


Figure 2.34: The Resource Inventory Data dialog.

Next, click the **Chart Style** button to bring up the 'Inventory Chart Style' dialog. Switch to the 'Time Line' tab and click the **Edit** button. In the 'Default Time Line Style' dialog that comes up, first select **Customize** under the 'Style Definition' section. Then change the minor time units count to 12 hours (the recipe cycle time) and click **OK** to return to the previous dialog. This will make observation of batches easier since a new batch cycle starts every 12 hours in this example. Click **OK** again to continue and the chart will be displayed with several batches. Set the number of batches to 12 by right-clicking on the chart and selecting **Set**

Number of Batches from the context menu that pops up. The resulting chart will look like that of Figure 2.35.

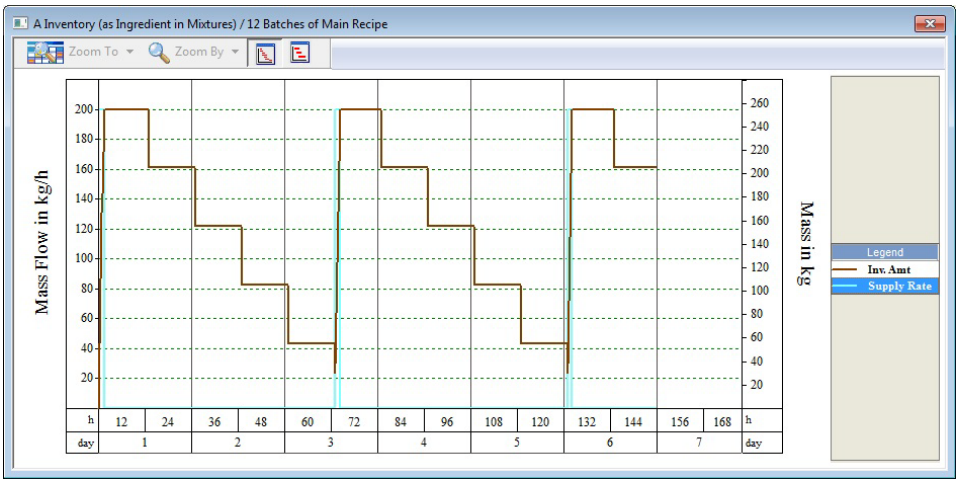


Figure 2.35: The inventory profile of pure component 'A' in the example.

The brown line in Figure 2.35 corresponds to the inventory level and the aqua line corresponds to the supply rate of material 'A'. The increases in inventory indicate the replenishment schedule suggested by SuperPro Designer.

To explain this further, let us focus on the first batch cycle. Please click the **Show Chart at Nominal Size** button ( ) and then the **Zoom To** button (Zoom To) on the chart's toolbar and check the **Day** option. The chart will zoom to one day (see Figure 2.36). Notice that the supply of fresh material starts right away since the opening inventory (100 kg) is less than 85% of storage capacity (255 kg). The inventory amount increases linearly up to the point that a charge of material starts as part of operation 'Charge React A' (45 minutes into the process). During that operation, 50 kg of material are being discharged to the process, and at the same time fresh material is still being supplied to the inventory tank (at a higher rate than the discharge associated with the charge operation). This results in a smaller rate of increase in the inventory amount during the 30 minutes that the charge operation is occurring. Afterwards, the inventory amount increases at the original rate again until it reaches the 85% limit, which triggers material supply off. The inventory amount remains at the same level until new material is discharged to the process roughly 12 hours later. In subsequent batch cycles, every time material is charged, the inventory amount falls by 50 kg. This leaves 55 kg in inventory at the beginning of the sixth batch cycle. During the charge operation in that cycle, the inventory amount reaches 10% of storage capacity (30 kg), which triggers the supply of fresh material on, while the charge of material to the process is on-going (please scroll to the 3rd day of the chart to observe this). This results in a modest increase in the inventory amount during the final part of the charge operation in the sixth batch cycle. After the charge operation is completed, the inventory amount increases at a higher rate until it reaches 85% of storage capacity and

material supply is triggered off again. The above replenishment schedule is repeated every sixth batch cycle.

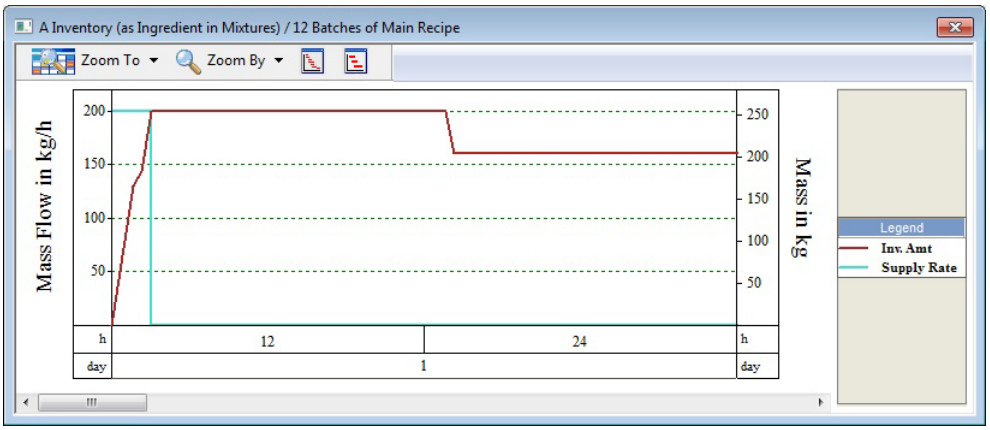


Figure 2.36: The inventory profile of pure component 'A' during Day 1.

Note that you can see the exact time and value of a point in a line by placing the mouse pointer over that point. By default, the inventory graph displays the inventory amount and the supply rate. To change the contents (variables displayed) and style (e.g., color, thickness, time line units, etc.) of the graph, right-click on the chart to bring up its context menu and click **Edit Style**. Through other context menu commands, you can print a chart, export a chart as a Windows Metafile (.wmf), or export chart data into a file in Excel format with a discretization time interval that can be specified by the user. This is a useful feature if you wish to combine demands for a certain resource from multiple flowsheets in Excel.

2.1l Throughput Analysis and Debottlenecking

SuperPro Designer is equipped with powerful throughput analysis and debottlenecking capabilities. The objective of these features is to allow the user to quickly and easily analyze the capacity and time utilization of each piece of equipment, and to identify opportunities for increasing throughput with the minimum possible capital investment. The most important features are:

- the Utilization Factors chart, and
- the Batch Size Potential chart, which indicates opportunities for increased production per batch.

For a detailed throughput analysis example (based on the process of the second example), see Chapter 11 (Debottlenecking). A brief description is given here.

Since throughput calculations are based on fixed equipment, set all pieces of equipment to 'Rating Mode'. Specify a volume of 1630L for the reactor and an area of $2m^2$ for the filter (as was done for file 'GettingStarted9_0b' in subdirectory 'Examples\Misc') and solve the material and energy balances by selecting **Solve M&E Balances** on the **Tasks** menu or clicking the **Solve ME Balances** button ( ) on the **Main** toolbar.

UTILIZATION FACTORS CHART

Select **Throughput Analysis ▸ Utilization Indices** on the **Charts** menu. The Utilization Factors chart shown below will appear.

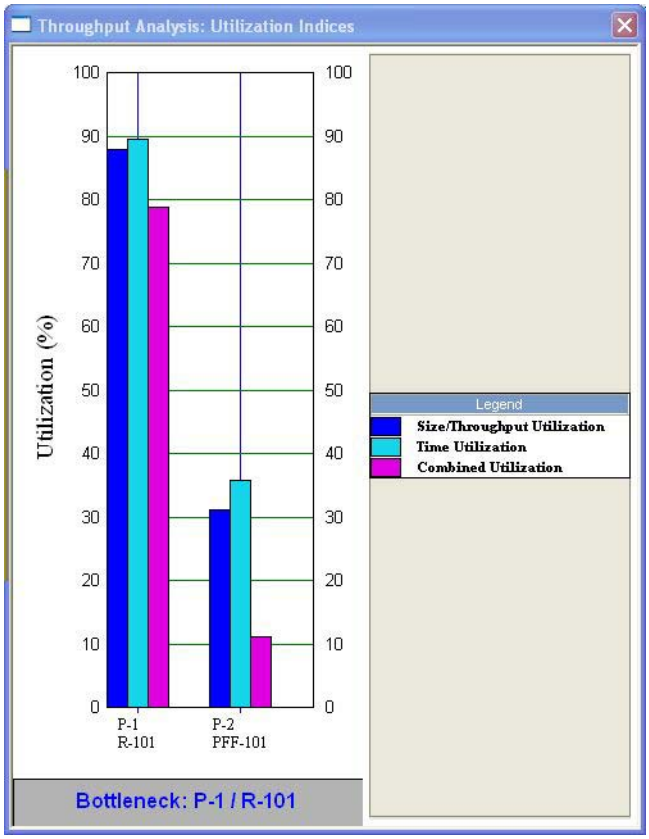


Figure 2.37: The Utilization Factors Chart.

The chart shows, for each unit procedure, the capacity (size) utilization (i.e., how "full" the equipment is) and the time utilization (i.e., its "uptime" or "busy time") of the hosting equipment. This information is also available in the 'Throughput' tab of the 'Procedure Data' dialog for each unit procedure. Note that the time utilization is somewhat low because some slack time was introduced (see Figure 2.30). The "combined utilization" is the product of the capacity and time utilization values. A batch size (throughput) bottleneck corresponding to the limiting procedure/equipment combination in terms of highest combined utilization ('P-1/R-101' in this case) is also indicated on the chart.

BATCH SIZE POTENTIAL CHART

Furthermore, estimates of batch size (throughput) potential are available in the Batch Size Potential chart. To create this chart, you must first select a throughput reference rate for batch size calculations. Select **Tasks ▸ Rate Reference Flow(s)** to open the 'Rate Reference Flows' dialog and switch to the 'Throughput' tab. Select the 'Other' option for Stream and

Flow Basis and set the total flow of the ‘Cake’ stream as reference (see Figure 2.38). Then click **OK** to close this dialog.

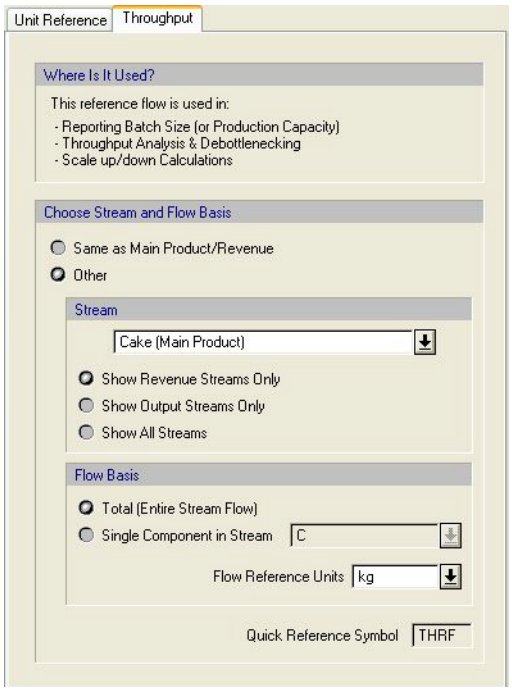


Figure 2.38: The Rate Reference Flows dialog.

Subsequently, select **Throughput Analysis ▸ Batch Size Potential** on the **Charts** menu to view the batch size potential chart using the total flow of the ‘Cake’ stream as the throughput reference rate (see Figure 2.39). This chart shows the actual batch size (red dotted lines) and three estimates (conservative, realistic, and theoretical) of batch size potential for each procedure/equipment combination. A size bottleneck based on each estimation method is also indicated on the chart. This corresponds to the procedure/equipment combination that has the smallest batch size potential based on that method. In this example, ‘P-1/R-101’ is the size bottleneck based on any estimation method. For each unit procedure, the above information can also be found in the ‘Throughput’ tab of the corresponding simulation data dialog.

To omit an equipment resource from the throughput analysis and, thereby, from the above charts, open the corresponding ‘Equipment Data’ dialog, switch to the ‘Throughput’ tab, and check the option named ‘Omit from Throughput Analysis’. For display purposes, a relevant

specification setting will be checked in the 'Throughput' tab of all unit procedures that utilize that equipment resource.

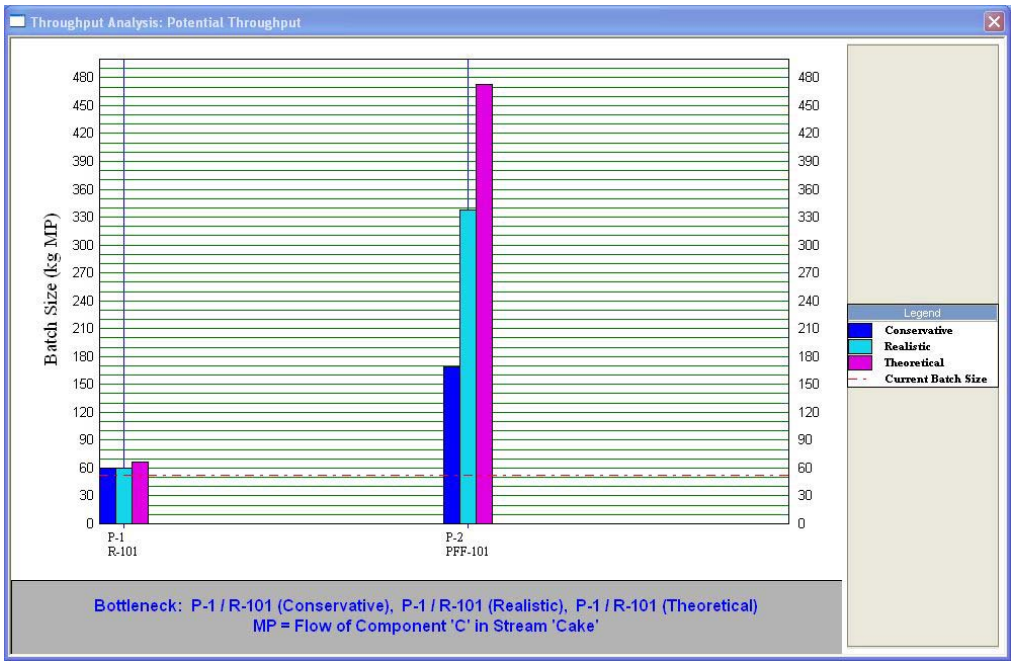


Figure 2.39: The Batch Size (Throughput) Potential Chart.

2.1m Cost Analysis and Economic Evaluation

SuperPro Designer performs thorough cost analysis and economic evaluation calculations and generates three pertinent reports. The key initialization steps are described below using our simple process as an example (see file 'GettingStarted9_0b' in the 'Examples\Misc' subdirectory of SuperPro Designer).

For a detailed descriptions of cost analysis and economic evaluation, please consult Chapter 9 (Economics).

SUPPLYING REVENUE, RAW MATERIAL, AND WASTE STREAM DATA

This step must precede economic evaluation and environmental impact assessment calculations. Please select **Stream Classification** on the **Task** menu. You will be presented with a dialog window (see Figure 2.40) where you can classify all input and output streams as raw materials, revenues or wastes (solid, aqueous, organic, or gaseous) and supply any cost data associated with the classification. By default, the system estimates a purchase or selling price for a stream based on the price of each component and the composition of the stream. The

price of a pure component or stock mixture is part of its properties, which can be edited when registering components as described in 2.1e Registering Components and Mixtures.

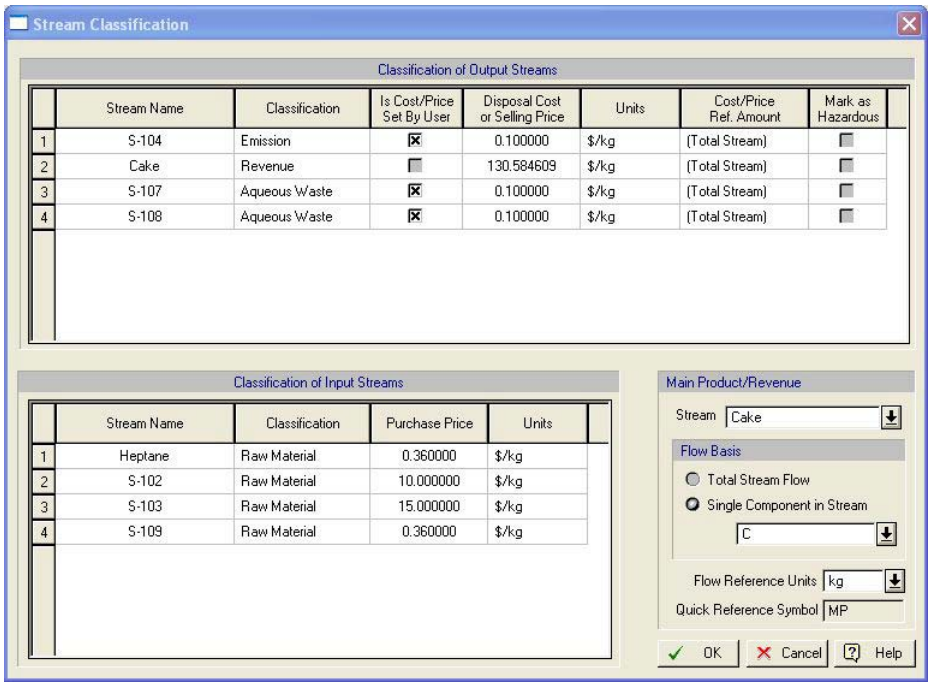

Stream Classification
Classification of Output Streams
Stream Name | Classification | Is Cost/Price Set By User | Disposal Cost or Selling Price | Units | Cost/Price Ref. Amount | Mark as Hazardous
1 S-104 Emission $ 0.100000 $/kg (Total Stream)
2 Cake Revenue 130.584609 $/kg (Total Stream)
3 S-107 Aqueous Waste $ 0.100000 $/kg (Total Stream)
4 S-108 Aqueous Waste $ 0.100000 $/kg (Total Stream)
Classification of Input Streams
Stream Name | Classification | Purchase Price | Units
1 Heptane Raw Material 0.360000 $/kg
2 S-102 Raw Material 10.000000 $/kg
3 S-103 Raw Material 15.000000 $/kg
4 S-109 Raw Material 0.360000 $/kg
Main Product/Revenue
Stream Cake
Flow Basis
Total Stream Flow
Single Component in Stream
C
Flow Reference Units kg
Quick Reference Symbol MP
OK
Cancel
Help

Figure 2.40: The ‘Stream Classification’ dialog.

In this example process, please classify the streams and set costs for the waste streams as shown in Figure 2.40. To to this, first specify that the ‘Cake’ stream is a revenue stream. Notice that the ‘Selling Price’ of a revenue stream is calculated automatically, based on the stream’s composition (recall that there is still heptane and small amounts of impurities in our product cake, so the price per kg of cake is less than the $200/kg price of pure component ‘C’.) Next, classify S-107 and S-108 as aqueous waste, and S-104 as an emission stream. Then check the ‘Set By User’ options next to the emission stream and the two liquid waste streams and type in a value of $0.10/kg for the ‘Disposal Cost’ of each. Finally, select the ‘Cake’ stream as the ‘Main Product/Revenue’ stream from the corresponding drop-down list in the lower right corner, and specify that the unit cost for this process will be reported based on the component flow of product ‘C’.

Note that the classification of a stream as a solid waste, aqueous waste, organic waste, or an emission will cause it to be reported in dedicated sections of the Environmental Impact Report, where a detailed bookkeeping is kept on all chemicals that end up in each waste category. Specifically, streams that are connected to venting ports are already classified as emission streams by default. The Environmental Impact Report allows you to evaluate the burden of the process on the environment. Such an assessment assists the designer to focus his/her attention on the most troublesome streams and the processing steps that generate them. A related report, the Emissions Report (EMS) provides information on emissions of volatile organic compounds (VOC) and other regulated compounds. The Emissions Report will also give information on the

emitted components as well as the contributing unit procedures and operations to these emissions.

ADJUSTING THE COST FACTORS

The user can specify economic evaluation parameters at four levels:

- the Operation level,
- the Equipment level,
- the process Section level, and
- the Process level.

Please note that the economic evaluation parameters from each of the three levels have a significant impact on the cost calculations. Therefore, the parameters at all three levels should be examined by the user and edited if necessary.

ECONOMIC PARAMETERS AT THE OPERATION LEVEL

Parameters that affect demand for labor and utilities are specified at the operation level. For instance, the labor requirement for an operation can be specified through the 'Labor, etc.' tab of an operation's data dialog. Through the same dialog you can also specify auxiliary utilities, which have no impact on process material and energy balance calculations (they do not affect output stream temperatures). Auxiliary utilities are only considered in costing and economic evaluation calculations. Auxiliary utilities offer a convenient way to associate utility consumption with generic boxes and other operations that do not calculate utility demand.

ECONOMIC PARAMETERS AT THE EQUIPMENT LEVEL

All equipment resources have two common dialog tabs through which the user can provide information that affects the capital investment and certain operating cost items. Information about equipment purchase costs and various adjustments can be provided through the 'Purchase Cost' and 'Adjustments' tabs of the 'Equipment Data' dialog.

Equipment Purchase Cost

Figure 2.41 shows the 'Purchase Cost' tab for Stirred Reactor (CSTR) 'R-101' in the example. To view this tab, right-click on vessel procedure 'P-1' and select **Equipment Data** on the context menu of that procedure. By default, SuperPro Designer uses a built-in model to estimate purchase costs for each piece of equipment. However, you can override this estimate by either using your own model or specifying an exact purchase cost (from a vendor quote, for instance).

Notice that the cost in Figure 2.41 has been adjusted for year 2011. To change the year of analysis for equipment cost calculations please see "Economic Evaluation Parameters Dialog:

Time Valuation Tab" within section 9.10a Economic Evaluation Parameters for Entire Project Dialog.

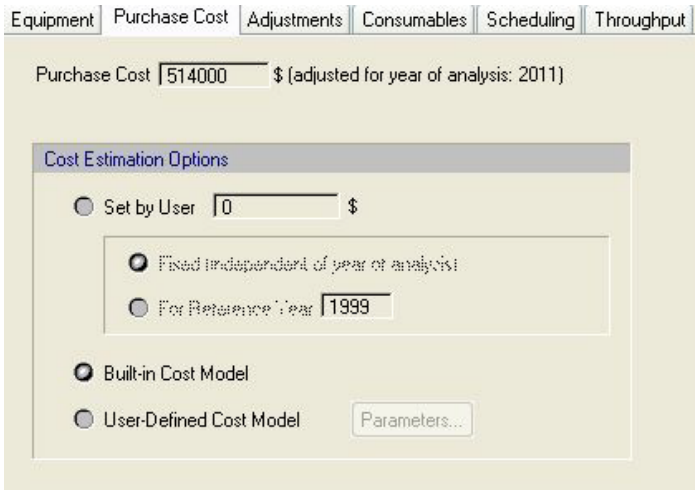


Figure 2.41: The 'Purchase Cost' tab of the 'Equipment Data' dialog.

Adjustments

Now please click on the 'Adjustments' tab of this dialog to view the number of standby units, the material, installation and maintenance cost factors, the percentage of purchase cost that is already depreciated, and the usage and availability rates for the batch reactor. The fields on this tab are described in detail below:

Number of Standby Units: For pieces of equipment that are critical to the operation of a process, you may choose to have one or more standby units (in case the regularly used pieces of equipment go down for scheduled or unscheduled maintenance). The number of standby units affects the capital investment but has no impact on maintenance and labor cost.

Material Factor: The purchase cost that is estimated using the built-in model corresponds to a certain material of construction that is displayed on this tab. Selecting a different material will affect the equipment purchase cost. The material cost factors for each type of equipment can be viewed by selecting **Equipment Materials** on the **Databanks** menu. Additional materials and material factors can be added to the 'User' database.

Installation Cost Factor: This factor is used to estimate the installation cost for each piece of equipment as a fraction of their purchase cost. The most common value is 0.3, meaning that the installation cost is 30% of the equipment purchase cost.

Maintenance Cost Factor: This factor is used to estimate the annual maintenance cost for each piece of equipment. The most common value is 0.1, meaning that the annual maintenance cost is 10% of its purchase cost.

Portion of Purchase Cost Already Depreciated: Oftentimes, a piece of equipment has already been either fully or partially depreciated. This can be captured using this variable. Any values other than 0.0% reduce the cost of depreciation but have no impact on the maintenance cost because that cost depends on the full purchase cost and not just the un-depreciated portion.

Usage and Availability Rates: These factors represent the equivalent of equipment rental rates. They are optionally used to estimate the Facility-Dependent (overhead) cost. For a description of this cost, see Chapter 9 (Economics).

If a piece of equipment is shared by multiple unit procedures, its purchase cost-dependent expenses (e.g., depreciation, maintenance, etc.) are distributed to its hosting steps based on the occupation time of each step.

Cost of Consumables

Consumables include materials and items that need to be replaced periodically, such us chromatography resins, cartridges of membrane filters, lubricants of equipment, etc. Items such as plastic bags, plastic bioreactors, roller bottles, etc. that are used once and thrown away belong to this category too. Parameters related to amount and frequency of consumption are specified through the Equipment Data Dialog: Consumables Tab. SuperPro Designer features a Consumables databank where users can store information for all consumables that they utilize. The information in the Consumables Databank can be viewed by selecting **Databanks ▸ Consumables...**.

ECONOMIC PARAMETERS AT THE SECTION LEVEL

Division of a process into sections facilitates reporting of results for economic evaluation, raw material requirements, and throughput analysis of integrated processes. A process section is a group of unit procedures that have something in common. All processes initially contain one section (called the 'Main Section' by default). For information on how to create process sections and edit their properties, see 2.2b Specifying Process Sections.

Section-level Capital Investment Factors

SuperPro Designer uses a factor-based method to estimate the capital investment associated with each section of a process. These factors have been assigned default values that should be reasonable for most cases. However, you should still check these factors to ensure that they are accurate for your situation. You can then adjust the factors to better suit your particular process file. Figure 2.42 shows the 'DFC' tab of a section's 'Capital Cost Adjustments' dialog. This tab allows you to edit factors used to estimate the direct fixed capital (DFC) of a section. The 'Capital Cost Adjustments' dialog is brought up by selecting the appropriate section ('Main Section' in this case) in the relevant drop-down list box on the 'Section' toolbar, and then clicking on the **Capital Cost Adjustments** ( ) button on the same toolbar. Alternatively, you may click **Process Options ▸ Section: <section name> ▸ Capital Cost Adjustments** on the **Edit** menu, or you can right-click on the flowsheet to bring up its context menu and then click **Section: <section name> ▸ Capital Cost Adjustments** (note that the term in brackets represents the name of the selected section).

The 'Distributed Set of PC-Factors' in the 'DFC' tab and the 'Startup and Validation Cost' factor in the 'Misc' tab can also be retrieved from a database site by allocating one or more process sections to that database site.That is the best way to utilize meaningful parameters for different industries around the globe. It is also the recommended way for standardizing cost analysis assumptions. For more information on how to take advantage of the database capabilities of SuperPro Designer for cost analysis, please consult the 'SynPharmDB' readme file in the 'Examples\SynPharm' directory of SuperPro Designer. Also, see 15.13 Sites & Resources Databank.

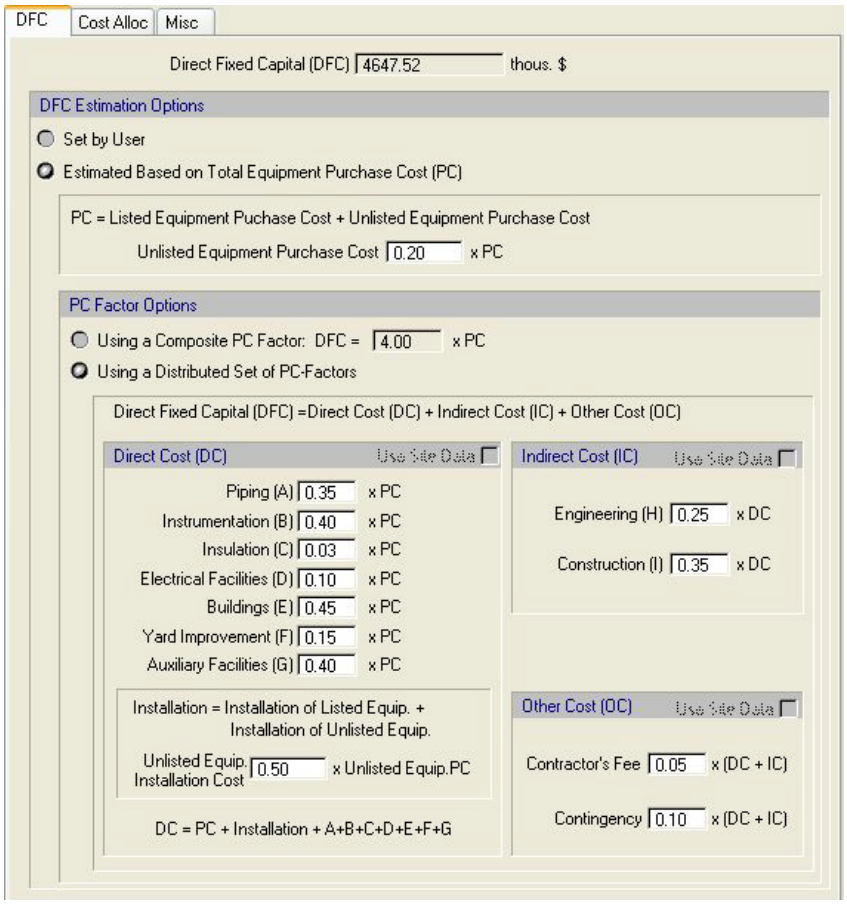

DFC
Cost Alloc
Misc
Direct Fixed Capital (DFC) 4647.52 thous. $
DFC Estimation Options
Set by User
Estimated Based on Total Equipment Purchase Cost (PC)
PC = Listed Equipment Puchase Cost + Unlisted Equipment Purchase Cost
Unlisted Equipment Purchase Cost 0.20 x PC
PC Factor Options
Using a Composite PC Factor: DFC = 4.00 x PC
Using a Distributed Set of PC-Factors
Direct Fixed Capital (DFC) =Direct Cost (DC) + Indirect Cost (IC) + Other Cost (OC)
Direct Cost (DC)
Use Site Data
Piping (A) 0.35 x PC
Instrumentation (B) 0.40 x PC
Insulation (C) 0.03 x PC
Electrical Facilities (D) 0.10 x PC
Buildings (E) 0.45 x PC
Yard Improvement (F) 0.15 x PC
Auxiliary Facilities (G) 0.40 x PC
Installation = Installation of Listed Equip. + Installation of Unlisted Equip.
Unlisted Equip. Installation Cost 0.50 x Unlisted Equip.PC
DC = PC + Installation + A+B+C+D+E+F+G
Indirect Cost (IC)
Use Site Data
Engineering (H) 0.25 x DC
Construction (I) 0.35 x DC
Other Cost (OC)
Use Site Data
Contractor's Fee 0.05 x (DC + IC)
Contingency 0.10 x (DC + IC)

Figure 2.42: Adjusting the capital cost parameters at the section level.

Section-level Operating Cost Factors

SuperPro Designer calculates and reports nine cost items for each process section: Materials, Labor-Dependent, Facility-Dependent, Laboratory/QC/QA, Consumables, Waste Treatment/Disposal, Utilities, Transportation, and Miscellaneous Costs. Figure 2.43 displays the options available for calculating the facility-dependent operating cost.

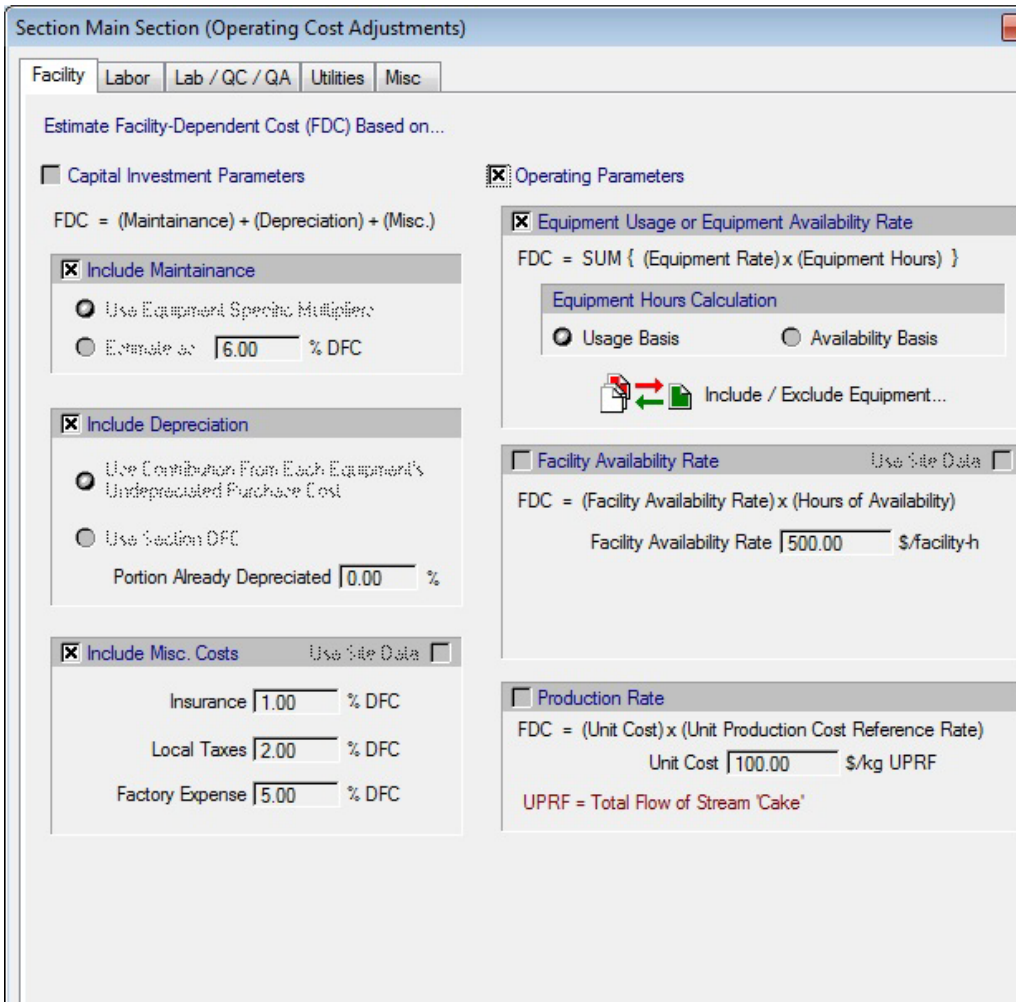

Section Main Section (Operating Cost Adjustments)
Facility
Labor
Lab / QC / QA
Utilities
Misc
Estimate Facility-Dependent Cost (FDC) Based on...
Capital Investment Parameters
Operating Parameters
FDC = (Maintainance) + (Depreciation) + (Misc.)
Include Maintainance
Use Equipment Specific Multipliers
Estimate as 6.00 % DFC
Include Depreciation
Use Contribution From Each Equipment's Undepreciated Purchase Cost
Use Section DFC
Portion Already Depreciated 0.00 %
Include Misc. Costs
Use Site Data
Insurance 1.00 % DFC
Local Taxes 2.00 % DFC
Factory Expense 5.00 % DFC
Equipment Usage or Equipment Availability Rate
FDC = SUM { (Equipment Rate) x (Equipment Hours) }
Equipment Hours Calculation
Usage Basis
Availability Basis
Include / Exclude Equipment...
Facility Availability Rate
Use Site Data
FDC = (Facility Availability Rate) x (Hours of Availability)
Facility Availability Rate 500.00 $/facility-h
Production Rate
FDC = (Unit Cost) x (Unit Production Cost Reference Rate)
Unit Cost 100.00 $/kg UPRF
UPRF = Total Flow of Stream 'Cake'

Figure 2.43: Adjusting the operating cost parameters at the section level.

This dialog is brought up by selecting the appropriate section ('Main Section' in this case) in the 'Section Names' drop-down list that is available on the **Section** toolbar and then clicking **Operating Cost Adjustments** ( ) on the same toolbar. Alternatively, you may select **Process Options ▸ Section: <section name> ▸ Operating Cost Adjustments** on the **Edit** menu, or you can right-click on the flowsheet to bring up its context menu and select **Section: <section name> ▸ Operating Cost Adjustments** (note that the term in brackets represents the name of the selected section). Through the 'Operating Cost Adjustments' interface, the user can adjust parameters that affect the Facility, Labor, Lab/QC/QA, Utilities, and Miscellaneous costs of a section. In your example, please change the Facility Cost to be based on an Equipment Usage Rate. This will account for depreciation, maintenance, and miscellaneous equipment expenses. To do that, uncheck the default option entitled 'Based on Capital Investment Parameters' and check the option entitled 'Based on Operating Parameters',

as shown in Figure 2.43. Also make sure that the 'Usage Basis' option is selected for the calculation of equipment hours. The equipment usage or availability rates are equipment-dependent, they are initialized to $100/h, and they can be edited through the 'Adjustments' Tab of the Equipment Data dialog.

Next, please visit the other tabs on the above dialog to familiarize yourself with their functions. Notice that in the 'Labor' tab there are various options for specifying the labor costs of your process, including lumped and itemized estimates for the labor hours and labor cost rate. Furthermore, the 'Lab/QC/QA' tab allows you to specify information for a detailed calculation of laboratory, quality control and quality assurance expenses. For more details on this, see Chapter 9 (Economics). After you are done, click **OK** to apply the changes made to this dialog and return to the flowsheet.

ECONOMIC EVALUATION FACTORS AT THE PROCESS LEVEL

Finally, there are parameters at the process level that affect the results of project economic evaluation. These are specified through the 'Economic Evaluation Parameters for Entire Project' dialog. This dialog box is brought up by selecting **Process Options ▸ Economic Evaluation Parameters** on the **Edit** menu (or, you can right-click on the flowsheet to bring up its context menu and select **Economic Evaluation Parameters**).

In the 'Time Valuation' tab (see Figure 2.44) of this dialog, the user can specify various time

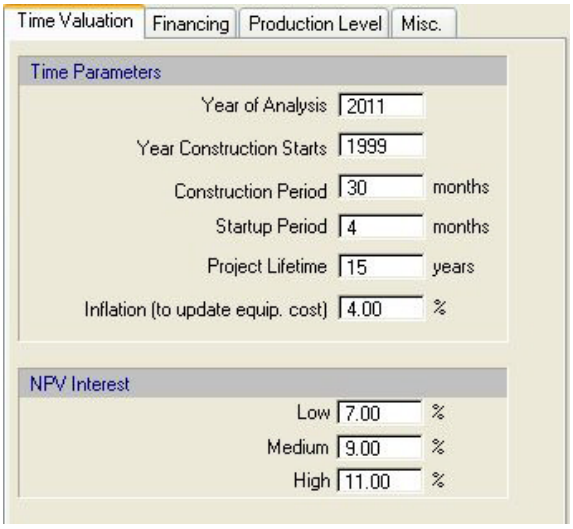


Figure 2.44: Adjusting the economic evaluation parameters at the process level.

parameters as well as the interest levels for calculating the net present value (NPV) of the project.

In the 'Financing' tab of the above dialog, the user can provide information on the financing of the project (e.g., equity versus borrowed money for DFC, working capital, etc.), the method of depreciation, the depreciation period, the salvage value and the DFC outlay (the spending of direct fixed capital as a function of time).

In the 'Production Level' tab of the above dialog, the user can specify the capacity utilization profile (production level) for the expected lifetime of the project and provide information for

product failure rate and disposal cost of scrapped product. Please note that the production level only affects the Cash Flow Analysis calculations. It has no impact on other project economic evaluation variables.

In the 'Miscellaneous' tab of the above dialog, the user can provide information for estimating income tax, advertising and selling expenses, and running royalties.

For the definitions of the different economic factors and for a description of how these are calculated, please consult Chapter 9 (Economics).

PERFORMING ECONOMIC CALCULATIONS AND VIEWING THE RESULTS

To ensure the financial sustainability of the process, select **Tasks ▸ Recipe Scheduling Information** and set the Calculated option for the Number of Batches per Year. After simulating the process, you can carry out the economic calculations by clicking **Perform Economic Calculations** on the **Tasks** menu. The same can be accomplished by clicking **Perform Economic Calculations** ( ) on the **Main** toolbar or pressing **Shift+F9** (hold down the **Shift** key and hit the **F9** key on your keyboard). Depending on your interest, you may then do the following:

1. View the equipment purchase cost for each process step. To do that, right-click on a desired unit procedure icon, select **Equipment Data** on the context menu of that procedure, and in the 'Equipment Data' dialog that appears switch to the 'Purchase Cost' tab. Remember that the displayed purchase cost is for a single piece of equipment. If the requirements to carry out the specific processing task are such that more than one equipment item (of the same size) is needed, the total cost is the indicated cost times the number of equipment items. The number of equipment items is displayed on the first tab of the 'Equipment Data' dialog.
2. Select **Executive Summary** on the **View** menu to view summary economic analysis results for the entire project. Please view the contents of the 'Executive Summary' dialog for your example process now. The corresponding 'Summary' tab in that dialog should look similar to Figure 2.45 shown below.
3. To view the detailed results which were used to produce the Executive Summary, you will need to generate the *Economic Evaluation Report* (EER). To generate and view this report, select **Economic Evaluation (EER)** on the **Reports** menu. Any report can be created in different file formats. You can set the format and many other settings from the dialog that comes up if you select **Options** on the **Reports** menu. The EER contains an executive summary that presents the key analysis results, a breakdown of the total capital cost, a breakdown of the annual operating cost and a description of profitability analysis calculations. Please generate and view the Economic Evaluation Report now.
4. Another useful economic report is the *Itemized Cost Report* (ICR). This report contains detailed cost breakdowns of the total annual operating cost over all process sections. This includes all cost items that are calculated at the section level. Additional cost items that are calculated at the process level are not considered. To generate this report, select **Itemized Cost (ICR)** on the **Reports** menu.
5. Finally, a *Cash Flow Analysis Report (CFR)* can be generated. This report includes loan information and detailed breakdowns of capital outlay, loan payment and cash flow for

each year over the expected lifetime of a project. To generate this report, select **Cash Flow Analysis (CFR)** on the **Reports** menu.

The equipment purchase cost shown in the 'Purchase Cost' tab of the 'Equipment Data' dialog corresponds to a single equipment unit.

For more information on the contents of the economic reports, please refer to the synthetic pharmaceutical example (see 2.2f Cost Analysis and Economic Evaluation), the β-Galactosidase example (see 2.3f Cost Analysis and Economic Evaluation) and the industrial wastewater treatment example (see 2.4c Cost Analysis and Economic Evaluation). For a detailed description of economic reports, see Chapter 12 (Reports).

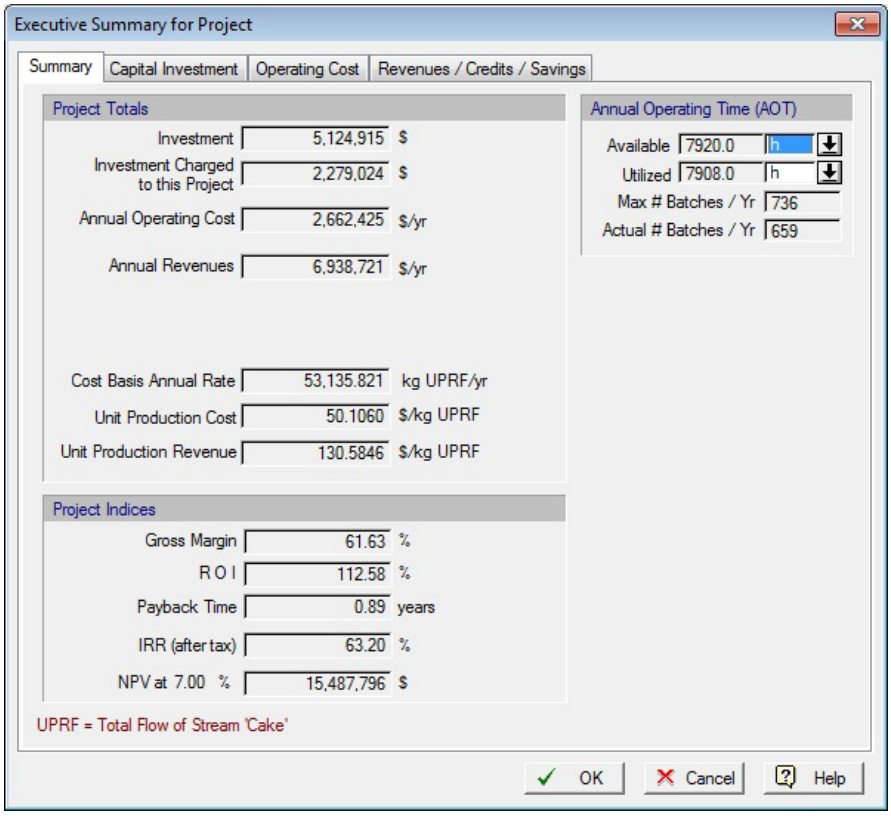

Executive Summary for Project
Summary
Capital Investment
Operating Cost
Revenues / Credits / Savings
Project Totals
Investment 5,124,915 $
Investment Charged to this Project 2,279,024 $
Annual Operating Cost 2,662,425 $/yr
Annual Revenues 6,938,721 $/yr
Cost Basis Annual Rate 53,135.821 kg UPRF/yr
Unit Production Cost 50.1060 $/kg UPRF
Unit Production Revenue 130.5846 $/kg UPRF
Annual Operating Time (AOT)
Available 7920.0 h
Utilized 7908.0 h
Max # Batches / Yr 736
Actual # Batches / Yr 659
Project Indices
Gross Margin 61.63 %
R O I 112.58 %
Payback Time 0.89 years
IRR (after tax) 63.20 %
NPV at 7.00 % 15,487,796 $
UPRF = Total Flow of Stream 'Cake'
OK
Cancel
Help

Figure 2.45: The 'Summary' tab of the 'Executive Summary' dialog for the example process.

2.1n Environmental Impact

SuperPro Designer generates two different reports that provide information on the environmental impact of a process. The Emissions Report (select **Emissions (EMS)** on the **Reports** menu) provides information on all emitted components including volatile organic compounds (VOCs) and other regulated compounds. The Environmental Impact Report (select **Environmental Impact (EIR)** on the **Reports** menu) provides information on the amount and type of waste generated by a manufacturing facility. It also provides information on the fate

of a compound that enters an integrated manufacturing or waste treatment facility; for more details on these reports, see Chapter 12 (Reports).

2.2 THE SYNTHETIC PHARMACEUTICAL PROCESS

This example analyzes the production of a synthetic pharmaceutical intermediate, which is formed by condensation of quinaldine and hydroquinone. The objective is to demonstrate how SuperPro Designer can be used as a tool to assist with scaling up the available pilot plant process into a large-scale process and maximize capacity using the available equipment at the lowest possible cost. This example is recommended for users in the pharmaceutical, agrochemical, and specialty chemical industries.

The process file and readme files for this example can be found in the 'Examples\SynPharm' directory of SuperPro Designer. The following process files demonstrate equipment sharing within a process and scaling-up of a process:

1. *SPhr8_0a*: This file represents an existing pilot plant process, which will act as the starting point for the scale-up process. The equipment sizes reflect a pilot plant environment. Four main pieces of equipment are used to carry out the process: two reactors named 'R-101' and 'R-102' (1200 L each), a Nutsche filter named 'NFD-101' (1 m^2 filter area), and a tray dryer named 'TDR-101' (3 m^2 tray area). There is also a storage bin named 'SB-101' which is not considered to be limiting the process in any way due to its low cost. This file demonstrates how to specify process sections and also, how to specify equipment sharing and visualize that through the equipment occupancy chart (see 2.1k Viewing Scheduling, Equipment Utilization and Resource Tracking Results).
2. *SPhr8_0b*: In this file, large-scale equipment is used while the process is still at the pilot plant scale.
3. *SPhr8_0c*: This file is based on the previous one. The process is scaled up to maximum batch size based on the limit imposed by equipment resource 'NFD-101' utilized by procedure 'P-3', and, more specifically, by the depth of the filter cake.

Once the process is scaled up, several strategies are evaluated on how to increase the process throughput. The following SuperPro Designer files analyze the strategies implemented in this case and demonstrate how to access the pertinent SuperPro Designer features in order to perform a similar exercise:

4. *SPhr8_0d*: This file demonstrates how to eliminate an equipment *size bottleneck* (an equipment resource that limits the batch size of the process) by increasing its time utilization. In this case, equipment 'NFD-101' utilized by procedure 'P-3' is the size bottleneck (imposed by the depth of its cake) but it is underutilized in time. By increasing the number of cycles per batch for procedure 'P-3' from 1 to 2, shifts the size bottleneck to equipment 'R-102' utilized by procedure 'P-10'. Equipment 'R-102' is also the *scheduling bottleneck* (an equipment resource that limits the annual number of batches) in this example. This can be noted by viewing the equipment occupancy chart (see 2.1k Viewing Scheduling, Equipment Utilization and Resource Tracking Results).

5. *SPhr8_0e*: It was mentioned in the previous file that the new size and time bottleneck is equipment 'R-102'. In this file, an extra reactor is added to eliminate that bottleneck. As a consequence, the number of batches performed annually is increased and the scheduling bottleneck shifts to equipment 'NFD-101'. The above can be easily viewed with the help of the equipment occupancy chart (see 2.1k Viewing Scheduling, Equipment Utilization and Resource Tracking Results).
6. *SPhr8_0f*: Another filter is added in the same manner to the previous file to eliminate the new scheduling bottleneck and the annual number of batches is increased.
7. SPhr8_0g: This case is not as straightforward as the previous ones. It can be noted by looking at the utilization factors chart (see 2.1l Throughput Analysis and Debottlenecking) for the previous file that equipment resource 'R-103' utilized by procedure 'P-10' is the size bottleneck, while all other procedure/equipment combinations have modest size utilizations. In this case, the batch is split in two halves starting with procedure 'P-10'. That enables us to increase the batch size, but the number of batches per year drops. However, the increase in batch size overcompensates for the reduction in the number of batches.

For a detailed analysis of this example process using the above SuperPro Designer files, please refer to the 'Synpharm.doc' readme file that can be found in the same directory as the SuperPro Designer files.

2.2a Process Description

The description that follows refers to file SPhr8_0a. Please open this file now. The corresponding flowsheet for this file is shown in Figure 2.46. The following equipment is available:

- two Stirred Reactor (CSTR) vessels ('R-101' and 'R-102') each having a total volume of 1200 L,
- a Nutsche Filter ('NFD-101') with an area of 1 m^2,
- a Tray Dryer ('TDR-101') with a total tray area of 3 m^2, and
- a Solids Bin ('SB-101') of 82 L.

The generation of the process simulation was based on information available in the patent and technical literature. Several reaction and separation steps are required to synthesize and purify the product of this process. These steps are described below:

CHLORINATION REACTION - SALT FORMATION STEP ('P-1' IN 'R-101')

Unit procedure 'P-1' (a Batch Vessel Procedure in a Reactor) takes place in reactor 'R-101' and involves two reaction steps. The first reaction step (see Batch Stoichiometric Reaction operation named 'Chlorination Rxn') involves the chlorination of quinaldine. Quinaldine is dissolved in carbon tetrachloride (CCl_4) and reacts with gaseous Cl_2. The yield of the reaction is around 98% (see 'Reactions' tab for this operation). The generated HCl is neutralized using Na_2CO_3. The stoichiometry and yield data of the three reactions are as follows::

$$\text{Quinaldine} + Cl_2 \rightarrow \text{Chloroquinaldine} + HCl \qquad \text{Yield} = 98\%$$

$$Na_2CO_3 + HCl \rightarrow NaHCO_3 + NaCl \qquad \text{Yield} = 100\%$$

$NaHCO_3 + HCl \rightarrow NaCl + H_2O + CO_2$ Yield = 100%

Small amounts of unreacted Cl_2, generated CO_2, and gaseous CCl_4 are vented. The above three reactions occur sequentially in 'P-1'.

The second reaction step (see Batch Stoichiometric Reaction operation named 'Salt Formation') involves the formation of chloroquinaldine·HCl salt. The added HCl first neutralizes the remaining $NaHCO_3$ and then reacts with chloroquinaldine to form its salt. The stoichiometry and yield of the two reactions are as follows:

$NaHCO_3 + HCl \rightarrow NaCl + H_2O + CO_2$ Yield = 100%

$Chloroquinaldine + HCl \rightarrow Chloroquinaldine \cdot HCl$ Yield = 100%

Small amounts of generated CO_2 and gaseous CCl_4 are vented. The presence of water (added with HCl as hydrochloric acid solution) and CCl_4 leads to the formation of two liquid phases. The small amounts of unreacted quinaldine and chloroquinaldine remain in the organic phase while the salts chloroquinaldine·HCl and NaCl move to the aqueous phase. After the reaction, the contents are allowed to settle, and the aqueous phase is transferred to reactor 'R-102' for further processing (see Batch Extraction / Phase Split operation named 'Transfer Aqueous Phase'). The organic phase is then discharged as waste (see Transfer Out operation named 'Dispose Organic'). Approximately 11.3 hours are required for the chlorination and salt formation reactions above, along with all associated charges and transfers (note that the times given for other procedures below will also include associated material transfers, etc.). This is the cycle time for 'P-1'. This information is available in the 'Scheduling' tab of the simulation data dialog for this procedure. To open this dialog, right-click on the procedure icon and select **Procedure Data**.

CONDENSATION REACTION STEP ('P-2' IN 'R-102')

Unit procedure 'P-2' (a Batch Vessel Procedure in a Reactor) takes place in reactor 'R-102' and involves the condensation of chloroquinaldine and hydroquinone (see Batch Stoichiometric Reaction operation named 'Condensation Rxn'). First, the salt chloroquinaldine·HCl is converted back to chloroquinaldine using NaOH. Then, hydroquinone reacts with NaOH and yields hydroquinone·Na. Finally, chloroquinaldine and hydroquinone·Na react and yield the desired intermediate product. Along with product formation, a small amount of chloroquinaldine dimerizes and forms an undesirable by-product (pure component named 'Impurity') that needs to be removed from the product. The stoichiometry and yield of the four reactions are as follows::

$Chloroquinaldine \cdot HCl + NaOH \rightarrow NaCl + H_2O + Chloroquinaldine$ Yield = 100%

$2Chloroquinaldine + 2NaOH \rightarrow 2NaCl + 2H_2O + Impurity$ Yield = 2%

$Hydroquinone + NaOH \rightarrow Hydroquinone \cdot Na + H_2O$ Yield = 100%

$Chloroquinaldine + Hydroquinone \cdot Na \rightarrow NaCl + Product$ Yield = 100%

This step takes a total of approximately 11 hours.

FILTRATION STEP #1 ('P-3' IN 'NFD-101')

Unit procedure 'P-3' (a Nutsche Filtration Procedure) takes place in Nutsche filter 'NFD-101' and involves product recovery. Both the product and impurity molecules formed during the condensation reaction precipitate out of solution and are recovered using a Nutsche filter (see Cloth Filtration operation named 'Product Isolation'). The product recovery yield is 90%. The total filtration and cake discharge time (i.e., the procedure cycle time) is 4.9 hours assuming an average filtrate flux of 200 L/m^2-h.

SOLUBILIZATION REACTION STEP ('P-4' IN 'R-101')

Unit procedure 'P-4' (a Batch Vessel Procedure in a Reactor) takes place in reactor 'R-101' and involves a solubilization reaction step. The product/impurity cake recovered by filtration is added into a NaOH solution. The product molecules react with NaOH forming product·Na (see Batch Stoichiometric Reaction operation named 'Product Solubilization') which is soluble in water. The Impurity molecules remain in solid phase. The stoichiometry and yield of the solubilization reaction follows:

$$\text{Product} + \text{NaOH} \rightarrow \text{H}_2\text{O} + \text{Product} \cdot \text{Na} \qquad \text{Yield} = 100\%$$

This step takes a total of approximately 6.9 hours.

FILTRATION STEP #2 ('P-5' IN 'NFD-101')

Next, the impurity is removed using another filtration step that takes place in Nutsche filter 'NFD-101'. The total time for filtration, cake wash and cake discharge is around 3.2 hours using an average filtrate flux of 200 L/m^2-h.

PRECIPITATION REACTION STEP ('P-6' IN 'R-102')

Unit procedure 'P-6' (a Batch Vessel Procedure in a Reactor) takes place in reactor 'R-102' and involves a precipitation reaction step. The excess NaOH is neutralized using HCl and then product.Na is converted back to product (see Batch Stoichiometric Reaction operation named 'Precipitation Rxn'). The stoichiometry and yield of the two reactions are as follows:

$$\text{HCl} + \text{NaOH} \rightarrow \text{NaCl} + \text{H}_2\text{O} \qquad \text{Yield} = 100\%$$

$$\text{HCl} + \text{Product} \cdot \text{Na} \rightarrow \text{NaCl} + \text{Product} \qquad \text{Yield} = 100\%$$

The product, which is insoluble in water, precipitates out of solution. This step takes around 9.2 hours.

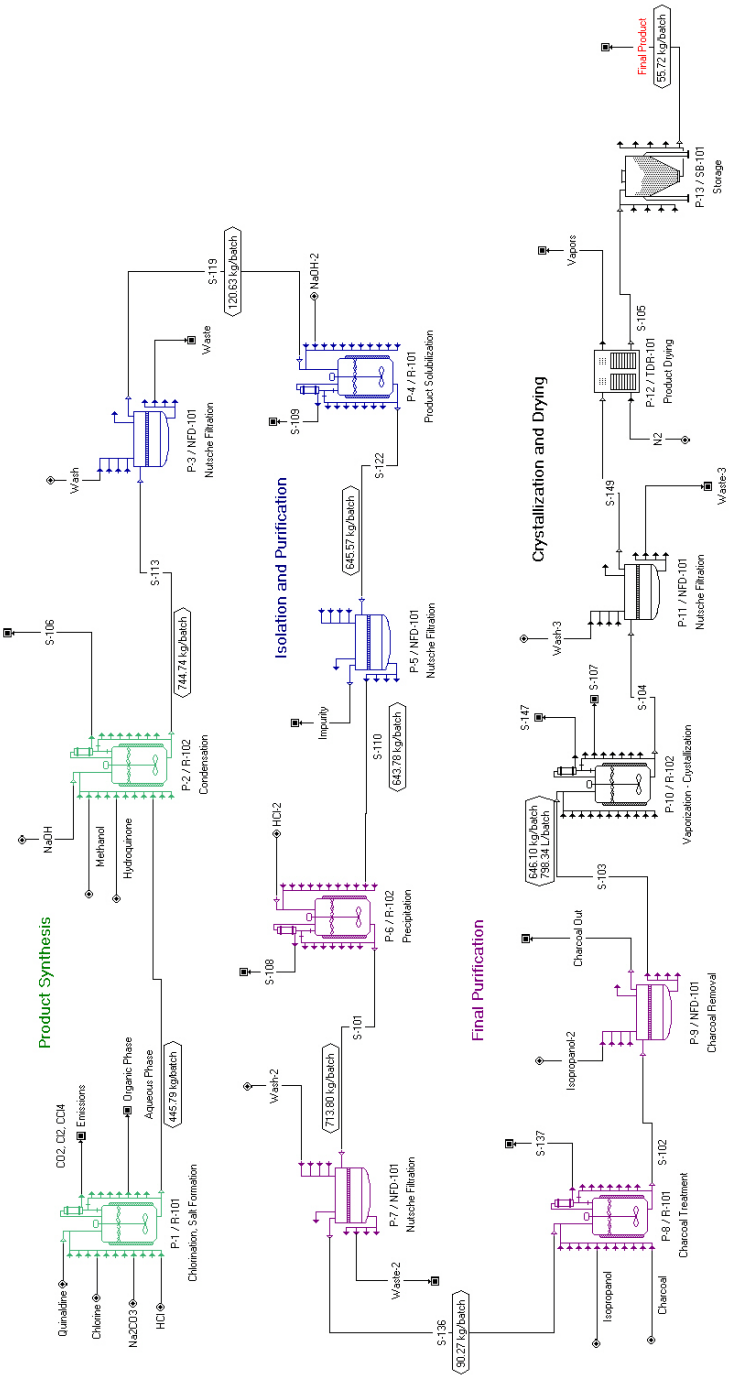


Figure 2.46: The process flowsheet for the synthesis of a pharmaceutical intermediate compound.

FILTRATION STEP #3 ('P-7' IN 'NFD-101')

Next, the product is recovered using another filtration step that takes place in Nutsche filter 'NFD-101'. The product cake is washed with water to remove impurities. The product recovery yield is 90%. The total time for filtration and cake discharge is around 4.4 hours using an average filtrate flux of 200 L/m^2-h.

CHARCOAL TREATMENT ('P-8' IN 'R-101')

Unit procedure 'P-8' (a Batch Vessel Procedure in a Reactor) takes place in reactor 'R-101' and involves charcoal treatment of the product cake. The recovered product cake is dissolved in isopropanol and treated with charcoal for removal of colorants. This step takes a total of approximately 13.5 hours.

FILTRATION STEP #4 ('P-9' IN 'NFD-101')

After charcoal treatment, the carbon particles are removed using another filtration step that takes place in Nutsche filter 'NFD-101'. The total time for filtration and cake discharge is around 4 hours using an average filtrate flux of 200 L/m^2-h.

VAPORIZATION - CRYSTALLIZATION STEP ('P-10' IN 'R-102')

Unit procedure 'P-10' (a Batch Vessel Procedure in a Reactor) takes place in reactor 'R-102' and involves two steps. First, the product solution is concentrated by vaporizing isopropanol (see Batch Vaporization / Solvent Switch operation named 'VAPORIZE-1'). During vaporization, the maximum working-to-vessel volume ratio is set to 70% (which also determines the size of the equipment). The reason behind this is the volume expansion that needs to be accounted for due to the gas formation. Vaporization operations generally require a lower working-to-vessel volume ratio than reaction operations. The 70% working-to-vessel volume ratio is used in all SuperPro Designer files included with this example. After vaporization, the product is crystallized with a yield of 97% (see Batch Stoichiometric Reaction operation named 'Crystallization'). Crystallization is represented by the following reaction:.

$$\text{Product} \rightarrow \text{Product-Cryst} \qquad \text{Yield} = 97\%$$

In other words, a new component ('Product-Cryst') is used to represent the crystalline form of product. This step is performed in approximately 10.9 hours.

FILTRATION STEP #5 ('P-11' IN 'NFD-101')

The crystalline product is recovered using another filtration step that takes place in Nutsche filter 'NFD-101' with a yield of 90%. The total time for filtration and cake discharge is around 2.8 hours using an average filtrate flux of 200 L/m^2-h.

DRYING STEP ('P-12' IN 'TDR-101')

In unit procedure 'P-12' (a Tray Drying Procedure), the recovered product crystals are dried in a tray dryer ('TDR-101'). The drying takes around 15.4 hours. Approximately 55.7 kg of dried product is produced per batch.

STORAGE (P-13 IN SB-101)

Finally, the dried process material is stored in a storage bin ('SB-101') during unit procedure 'P-13' (a Batch Solids Storage in a Bin Procedure).

2.2b Specifying Process Sections

A process section is a group of processing steps that have something in common. Many economic factors in SuperPro Designer are section-dependent and that is one reason to break-up your process into more than one sections. The process of this example was divided into four sections:

1. 'Product Synthesis' (green icons),
2. 'Isolation and Purification' (blue icons),
3. 'Final Purification' (purple icons), and
4. 'Crystallization and Drying' (black icons).

To create a new section, click **New Section** ( ) on the **Section** toolbar.

To add unit procedures to a specific section, first select the desired section in the 'Section Names' drop-down list that can be found on the 'Section' toolbar. Then, highlight the desired unit procedure icons on the flowsheet (use **Ctrl+Click** to add/remove unit procedures to/from the selection set) and click **Add to Section** ( ) on the same toolbar.

To rename the selected section, click **Rename Section** ( ) on the **Section** toolbar. To delete it, click **Delete Section** ( ) on the same toolbar. To access or modify the properties of a section (e.g., the color of unit procedure icons), click **Edit Section Properties** ( ) on the **Section** toolbar, or **Process Options** ▸ **Section: <section name>** ▸ **Properties** on the **Edit** menu (note that the term in brackets denotes the name of a selected section). This will bring up the properties dialog for the selected section. If you click on the 'Icon Color' tab of this dialog, you can edit the section's default unit procedure icon color.

Another reason to break-up a process in two or more sections is that you can allocate sections to different physical sites declared in the Sites and Resources databank (contained in the 'User' database) and thus make use of equipment and resources of specific sites. To use this feature, you will first need to declare the sites in the databank by selecting **Sites and Resources** on the **Databanks** menu. Through the dialog that comes up, you are able to define new sites in a parent-child hierarchy (i.e. sites with their sub-sites or facilities) and declare their equipment, utility and labor resources as well as site-related economic data (see 6.1i Equipment Allocation and 15.13 Sites & Resources Databank for details).

▶ To allocate a section to a site...

1. Select the desired section in the 'Section Names' drop-down list of the **Section** toolbar.
2. Click **Edit Section Properties** ( ) on the **Section** toolbar.
3. In the 'Allocation' tab, select the 'Allocated to database site' option, and then select the desired site from the drop-down tree that is available next to that option.
4. Click **OK** to close the dialog.

Once you allocate a section to a database site, you can allocate equipment of that section to site equipment and also make use within each operation of site utilities and labor.

For more information on how to allocate sections and equipment to database entities, please consult the 'SynPharmDB.doc' readme file that can be found in the 'Examples\SynPharm' directory of SuperPro Designer. See also 6.1i Equipment Allocation and 15.13 Sites & Resources Databank.

Following the instructions in the readme file and in 6.1i Equipment Allocation and 15.13 Sites & Resources Databank, you might want to go through the exercise of declaring a new site in the Sites & Resources databank and allocating one or more sections of this example to that site.

In the section properties dialog, you can also define and see the 'Starting Material' and 'Active Product' for a section along with the calculated yields. If you go to the 'Yields' tab, you can see the molar yield for each section. In this example, the molar yields of the 'Product Synthesis', 'Isolation and Purification', 'Final Purification', and 'Crystallization and Drying' sections are 93.9%, 89.9%, 90.0%, and 87.3%, respectively.

For more details on process sections, see 8.1 Sections & Branches or consult the Help documentation (look up the keyword 'Sections' in the Help index).

2.2c Specifying Equipment Sharing

It is important to understand that when you model batch processes in SuperPro Designer, the flowsheet depicts a representation of processing steps (unit procedures) and not a representation of equipment. This is the case because in a batch plant, it is common to utilize the same piece of equipment for carrying out multiple processing steps. In this example, for instance, the 'Chlorination, Salt Formation' ('P-1'), 'Product Solubilization' ('P-4') and 'Charcoal Treatment' ('P-8') steps share reactor 'R-101'. The 'Condensation' ('P-2'), 'Precipitation' ('P-6'), and 'Vaporization - Crystallization' ('P-10') steps share reactor 'R-102'. Finally, all five filtration steps ('P-3', 'P-5', 'P-7', 'P-9', and 'P-11') utilize the same Nutsche filter ('NFD-101'). Notice that a shared equipment indicator () is shown at the bottom left corner of the corresponding unit procedure icons to indicate that the above steps use shared equipment.

By default, whenever a unit procedure is introduced in the process, the system assumes that the procedure is carried out in its own piece of equipment. However, you also have the option of selecting one of the existing equipment items that are compatible with this procedure through the 'Equipment' tab of the 'Equipment Data' dialog (right-click on a unit procedure icon and select **Equipment Data**).

Figure 2.47 displays the 'Equipment' tab for procedure 'P-4'. Instead of using a unique vessel for this procedure, the user decided to reuse 'R-101', which also handles procedure 'P-1'. Please note that if the processing times of two procedures that share the same equipment overlap in time, SuperPro Designer will generate a warning. Also note that equipment sharing is available in equipment 'Design Mode' as well as 'Rating Mode'. Equipment sharing is also implied when two or more unit procedures use equipment allocated to the same site equipment. The site-equipment databank, therefore, provides you the means to declare that the same equipment is used for multiple tasks not only in the same recipe but across recipes as well.

When multiple unit procedures share a piece of equipment in 'Design Mode' (unspecified size), each procedure recommends its own sizing to achieve the necessary throughput and SuperPro Designer selects the maximum. For each unit procedure, if the calculated equipment size to achieve the necessary throughput exceeds the user-defined maximum size specification, then SuperPro Designer assumes multiple equipment items of the same size so that:

- the equipment size is smaller than or equal to the maximum size specification, and
- the total size of all equipment items is equal to the calculated total size requirement.

For example, if a maximum size of 5 m^2 is specified in 'Design Mode' for Nutsche filter 'NFD-101', and your process requires 12 m^2 of filter area to achieve the necessary throughput, three 4 m^2 filters will be used by SuperPro Designer.

In 'Rating Mode', the user specifies the equipment size as well as the number of equipment items employed by a unit procedure. In other words, in SuperPro Designer a single unit procedure icon may correspond to multiple equipment items that operate in parallel, or multiple unit procedure icons may correspond to a single piece of equipment (if the plant operation mode is batch and those procedures share equipment).

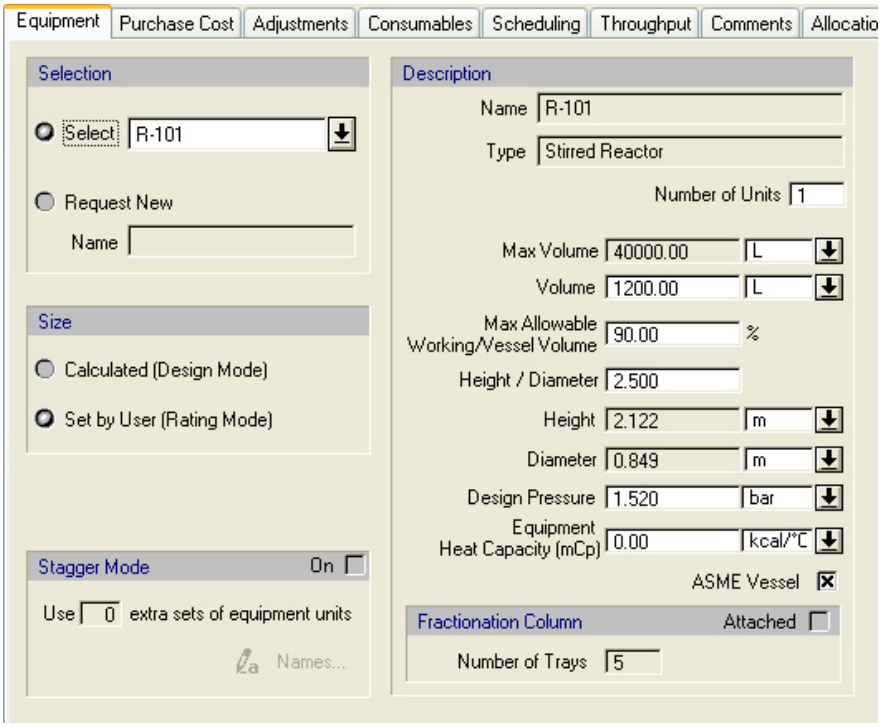


Figure 2.47: The 'Equipment' tab of the 'Equipment Data' dialog for unit procedure 'P-4'.

When the equipment is allocated to a site equipment, its size specification mode is set by default to 'Rating Mode' and the 'Design Mode' option is deactivated. In addition, all data specifications are copied from the site equipment and become non-editable. This signifies the fact that the equipment shown in the recipe is actually the one declared in the site databank and has therefore fixed specifications that cannot be changed unless you visit the site databank and change the specifications of the site equipment.

Equipment sharing reduces the number of equipment items required for a batch process and, consequently, saves money in terms of capital expenditures. However, it also introduces scheduling constraints that may reduce the number of batches that can be processed per year. For information on how to visualize equipment sharing, see 2.2e Process Analysis. For detailed information on the impact of equipment sharing on plant throughput, please consult Chapter 11 (Debottlenecking) or look up the keyword 'debottlenecking' in the Help documentation.

2.2d Initialization of Reaction Operations

Batch reactions constitute the most common operation in synthetic pharmaceutical processes. SuperPro Designer is equipped with three different batch reaction operation models:

- Batch Stoichiometric Reaction,
- Batch Kinetic Reaction, and
- Batch Equilibrium Reaction.

The stoichiometric is used if no kinetic and equilibrium data are available. If kinetic data are available, the kinetic model can be used to calculate composition, temperature, and utility profiles as a function of time. All reaction operations share the same 'Oper. Cond's' tab (see Figure 2.48) through which the user can specify the duration of the operation, the thermal mode, the power consumption, etc.

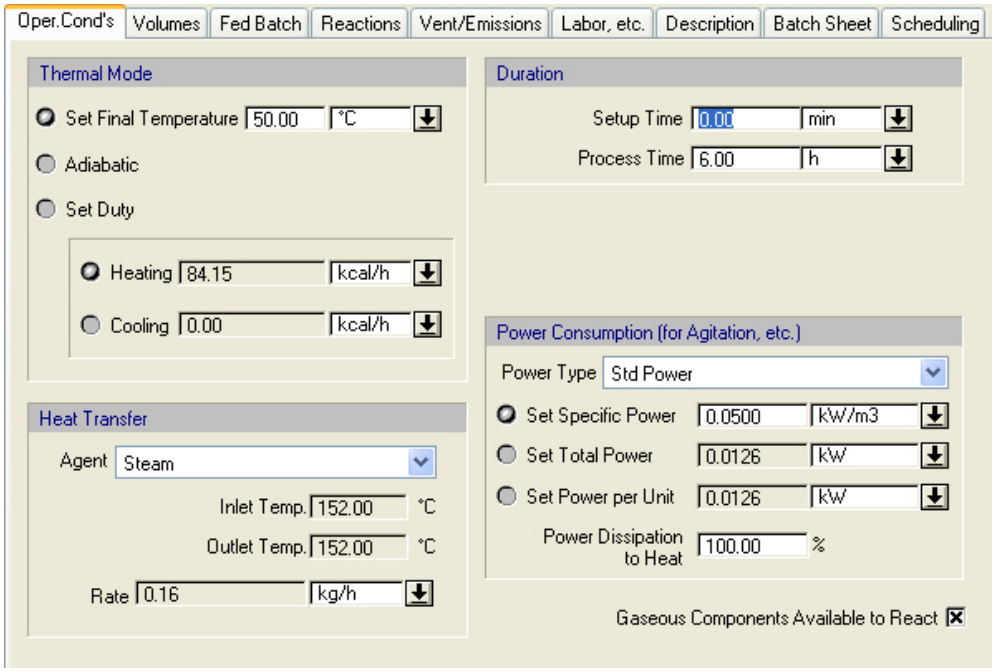


Figure 2.48: The 'Oper.Cond's' tab for the chlorination reaction operation i n procedure 'P-1'.

Similarly, all reaction operations share the same 'Volumes' tab (see Figure 2.49). In equipment 'Design Mode' (equipment size is unspecified), the maximum allowable working-to-vessel volume (%) specification is used for sizing the vessel. If multiple operations in the same unit procedure require different equipment capacities, the maximum capacity requirement of these operations is selected as the equipment size. In equipment 'Rating Mode' (equipment size is specified), the maximum allowable working-to-vessel volume (%) specification acts as a constraint and SuperPro Designer generates a warning when it is violated. The maximum

allowable working-to-vessel volume (%) specification also acts as a constraint. The same logic applies to other vessel operations.

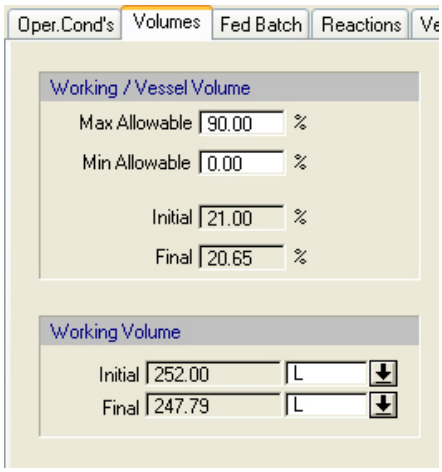


Figure 2.49: The 'Volumes' tab for the chlorination reaction operation i n procedure 'P-1'.

All batch reactions also have fed-batch capability for supply of additional reactants during the reaction operation. This is common practice in cases of highly exothermic reactions. Slow addition of one of the reactants controls the reaction rate and the need for cooling. Fed-batch operation is also common in bioprocessing to maintain a certain level of media concentration during fermentation.

For an example of a fed-batch reaction model, please consult example 'FedBR' in the 'Examples\Misc' directory of SuperPro Designer.

Figure 2.50 displays the 'Reactions' tab of a Batch Stoichiometric Reaction operation (in this case, 'Chlorination Rxn' in 'P-1'). Through this tab, the user specifies the stoichiometry and other data associated with the various reactions in this operation. Please note that a reaction operation can handle any number of reactions. The stoichiometry of a reaction is specified by selecting a reaction and clicking **Edit Stoichiometry** ( ). The 'Extent' of a stoichiometric reaction represents the fractional conversion of its limiting component. By default, the limiting component is identified by the model based on the stoichiometric coefficients and the feed composition. The user has the option to specify a reference component for the extent of reaction. In that case, if the specified reaction extent is not feasible, the model adjusts its value to the maximum possible. The user also has the option to specify the desired final concentration of a reactant or product and have the model estimate the extent of reaction. If the specified concentration is not feasible, the model adjusts its value to the maximum (or minimum) possible.

Several different methods can be used to specify multiple reactions within a single reaction operation. For instance, each reaction could be written individually, as was done for the 'Chlorination' and 'HCl Neutralization' reactions in Figure 2.50. The 'S' in the first column of the 'Reaction Sequence' listing indicates that the reactions take place sequentially (as opposed to 'P' for parallel reactions). In other words, first the 'Chlorination' reaction proceeds to its

specified reaction extent. Then, the first 'HCl Neutralization' reaction proceeds to its specified reaction extent. Finally, the second 'HCl Neutralization' reaction occurs. In other situations, you may wish to specify reactions that occur simultaneously. You can do this by clicking on the 'Parallel ?' check box for each reaction. In this case, the specified reaction extent for each reaction is applied to the material amounts as existing at the beginning of the parallel set of reactions. Note that you can have both sequential reaction steps and parallel groups of reactions in the 'Reaction Sequence' listing.

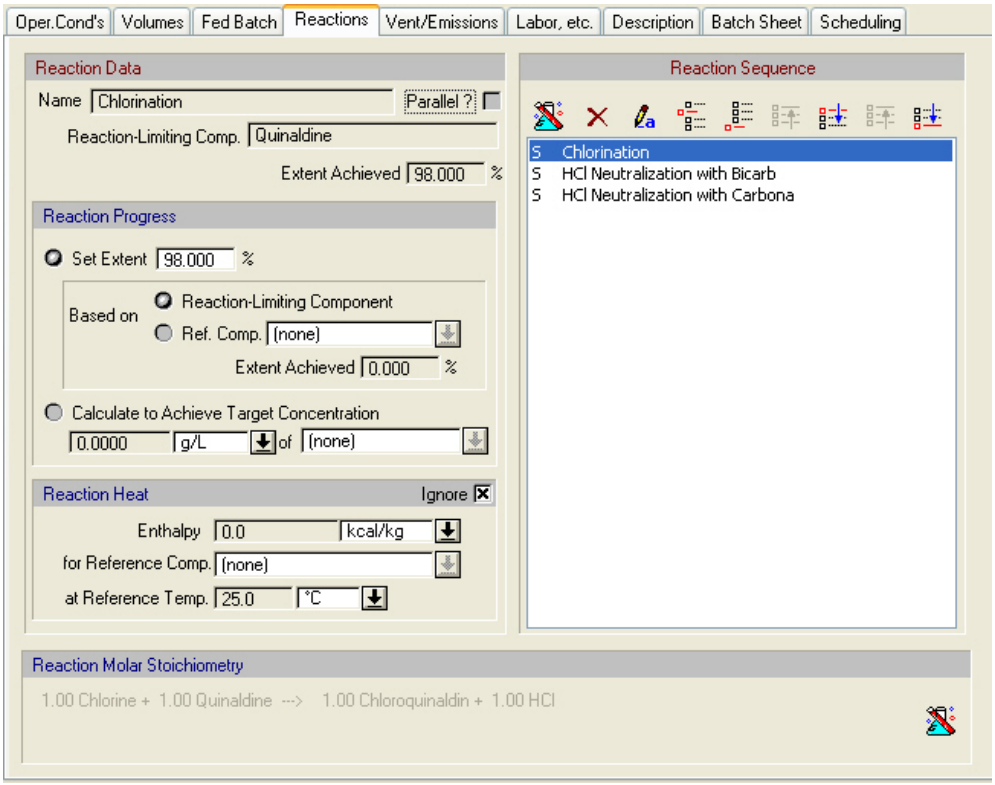


Figure 2.50: The 'Reactions' tab for the chlorination reaction operation i n procedure 'P-1'.

The 'Reactions' tabs of batch kinetic or equilibrium reactions is quite similar to that of Figure 2.50. The main difference is that instead of specifying the reaction extent, it has a button through which the user can bring up the kinetic data dialog for a reaction. Through this dialog, the user specifies the kinetics of a reaction. Furthermore, clicking on the 'Start/End Criteria' buttons brings up other dialogs through which the user can specify when or under what conditions a reaction is initiated or terminated. For more information on kinetic reactions, please consult examples 'BKinRxn', 'BKinFerm' and 'FedBR' in the 'Examples\Misc' directory of SuperPro Designer.

2.2e Process Analysis

At this point, you may return to the synthetic pharmaceutical example. Do not hesitate to change the values of certain parameters and redo the mass and energy balance calculations

(click **Solve ME Balances** ( ) on the **Main** toolbar or on the **Tasks** menu, or simply hit **Ctrl+3** or **F9** on your keyboard).

You can view the calculated flowrate and composition of intermediate and output streams by visiting the simulation data dialog of each stream (double click on a stream, or right-click on a stream and select **Simulation Data**). Alternatively, you may use the 'Stream Summary Table' to view selected attributes (e.g., total flow, temperature and pressure) of selected streams. To show or hide the 'Stream Summary Table', click **Stream Summary Table** ( ) on the **Main** toolbar. Figure 2.51 displays a portion of that table for this example.

		Time Ref: Batch		Aqueous Phase	Charcoal	Charcoal Out	Chlorine	Emissions
		Type			Raw Material	Solid Waste	Raw Material	Emission
		Total Flow	kg	445.7882	5.1000	8.3936	28.8000	20.2604
		Temperature	°C	50.00	25.00	42.44	25.00	20.00
		Pressure	bar	1.004	1.013	1.093	1.013	1.013

StreamSummary

Figure 2.51: Stream summary table displayed on the flowsheet.

Note that the 'Stream Summary Table' is empty when it is brought up the first time. To populate it, right-click on the table to bring up its context menu and select **Edit Contents**. This will bring up the 'Contents Selection' dialog, which allows you to specify which streams and stream attributes to monitor. You also have the option to exclude certain components from the list by clicking **Include / Exclude Components** ( ). In the table, you can choose different physical units for stream attributes by clicking on the physical units cells. The table can be floated by right-clicking on it to and checking the **Dock** option on the table's context menu. Also, the table has printing capabilities and can be easily exported to Excel. To print the table along with the flowsheet, the **Dock** and **Include in Printing** options on the table's context menu must be checked.

You may also generate the 'Streams & Material Balance (SR)' report by clicking **Streams & Mat. Balance (SR)** on the **Reports** menu. This report contains information on the overall process, raw material requirements, stream compositions and flowrates, as well as an overall material balance. You may customize the format and contents of this report through the 'Report Options' dialog. To open this dialog, select **Options** on the **Reports** menu. Please generate and view the 'Streams & Material Balance (SR)' report for this example now.

Figure 2.52 shows the overall process data table of the SR report for this example. MP stands for main product and it refers to the final dried crystals. It can be seen that around 55.7 kg of final dried crystals are produced per batch in this example. Also, the overall batch time (from start to finish of a single batch) is approximately 74 hours, whereas the time between two consecutive batch starts (the recipe cycle time) is approximately 50 hours.

Another table of the SR report is the starting material requirements table which is shown in Figure 2.53 for this process. The starting material and active product listed in this table for each section, are specified through the 'Yields' tab of a section's properties dialog. To view this dialog, first select the desired section in the 'Section Names' drop-down list that is available on the **Section** toolbar, and then click **Edit Section Properties** ( ) on the same toolbar.

Also, the bulk materials table of the SR report for this process is shown in Figure 2.54. This table provides information on raw material requirements for the entire process. Note that around 54.3 kg of materials (solvents, reagents, etc) are used per kg of main product produced in this example. Thus, the product-to-raw material ratio is only 2%, which indicates that this process generates large amounts of waste; for more details on the SR report, see 12.3 Material & Stream Report (SR).

1. OVERALL PROCESS DATA

Annual Operating Time	7,916.03h
Annual Production Rate	8,804.39kg MP
Batch Size	55.72kg MP
Recipe Batch Time	73.94h
Recipe Cycle Time	49.95h
Number of Batches per Year	158.00

MP = Total Flow of Stream 'Final Product'

Figure 2.52: The overall process data table of the Streams & Material Balance (SR) report.

2.1 STARTING MATERIAL REQUIREMENTS (per Section)

Section	Starting Material	Active Product	Amount Needed (kg Sin/kg MP)	Molar Yield (%)	Mass Yield (%)	Gross Mass Yield (%)
Product Synthesis	Quinaldine	Product	0.86	93.94	164.87	164.87
Isolation and Purification	Product	Product.Na	1.41	89.90	97.74	97.74
Final Purification	Product.Na	Product	1.38	90.00	82.78	82.78
Crystallization and Drying	Product	Product_crys	1.14	87.30	87.30	87.30

Sin = Section Starting Material, Aout = Section Active Product

Figure 2.53: The starting material requirements table of the Streams & Material Balance (SR) report.

2.2 BULK MATERIALS (Entire Process)

Material	kg/yr	kg/batch	kg/kg MP
Carb. TetraCh	25,280	160.000	2.871
Quinaldine	7,556	47.820	0.858
Water	184,090	1,165.125	20.909
Chlorine	4,550	28.800	0.517
Na2CO3	5,340	33.800	0.607
HCl (20% w/w)	18,170	115.000	2.064
NaOH (50% w/w)	10,396	65.800	1.181
Methanol	28,124	178.000	3.194
Hydroquinone	8,715	55.160	0.990
Sodium Hydroxid	3,770	23.860	0.428
HCl (37% w/w)	11,060	70.000	1.256
Isopropanol	113,467	718.145	12.888
charcoal	806	5.100	0.092
Nitrogen	56,449	357.274	6.411
TOTAL	477,774	3,023.885	54.265

Figure 2.54: The bulk material s table of the Streams & Material Balance (SR) report.

The detailed equipment contents during a processing step can be viewed by right-clicking on a desired unit procedure and selecting **Equipment Contents ▸ During <procedure name>** on the context menu of that procedure. Selecting **Procedure Activity Overview** on the same menu displays related information; for more details on viewing simulation results, see 2.1i Simulating the Process and Viewing the Simulation Results.

SCHEDULING, EQUIPMENT UTILIZATION, AND RESOURCE DEMAND GRAPHS

SuperPro Designer generates the Operations Gantt Chart and the Equipment Gantt Chart that display scheduling and equipment utilization information, respectively, for single or multiple batches. From the Gantt chart interfaces, you can also modify the scheduling parameters of unit procedures, operations, equipment (in Equipment Gantt Charts only), as well as of the entire recipe, and immediately visualize the effects on the entire batch production. A portion of the Operations Gantt Chart for this example and for a single batch is shown in Figure 2.55.

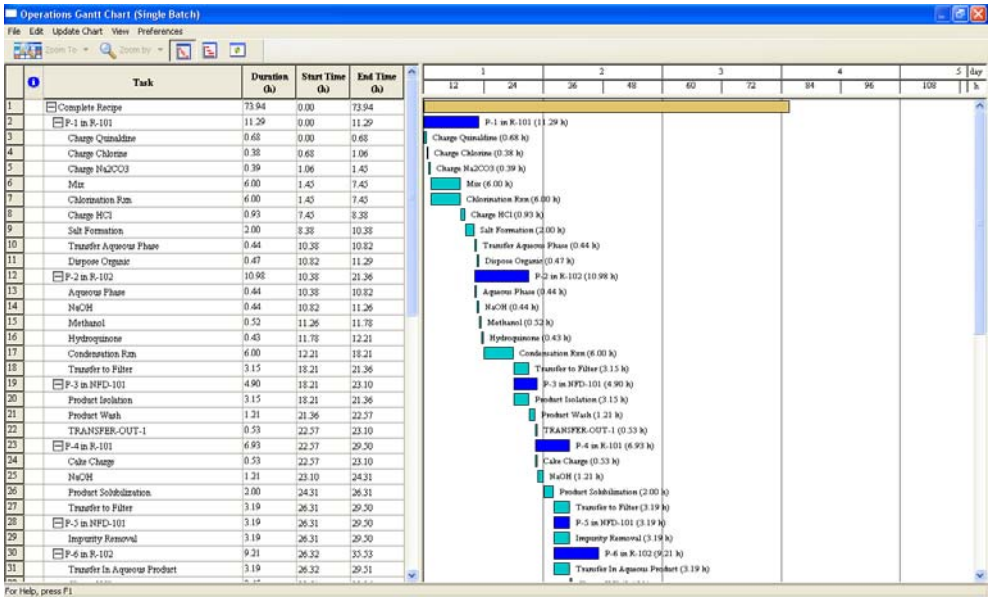


Figure 2.55: The Operations Gantt Chart for a single batch.

Another way of visualizing the execution of a batch process as a function of time is through the Equipment Occupancy Chart. This chart shows in a graphical way how long each equipment is kept busy by some operation and how long it is just idle during batch processing. The Equipment Occupancy Chart for two consecutive batches of this example process is shown in Figure 2.56. Please generate this chart now. To view scheduling summary information for this process on the chart (as was done in Figure 2.56), right-click on the chart to bring up its context menu and check **Scheduling Summary**. You may also access or modify the recipe scheduling information by selecting **Edit Recipe Scheduling Info** on the same menu.

As shown in this chart, Equipment 'R-101' is utilized by three different unit procedures ('P-1', 'P-4', and 'P-8') within a batch and some idle time exists between these procedures. This is indicated by the three blocks of the same color shown on the bar line of equipment 'R-101'. Each rectangle in a block represents a single operation. Placing the mouse pointer over a bar

displays the corresponding operation name and unit procedure name carried out in the host equipment at that time. Equipment items 'R-102' and 'NFD-101' also handle multiple processing steps (unit procedures) within a batch in this example.

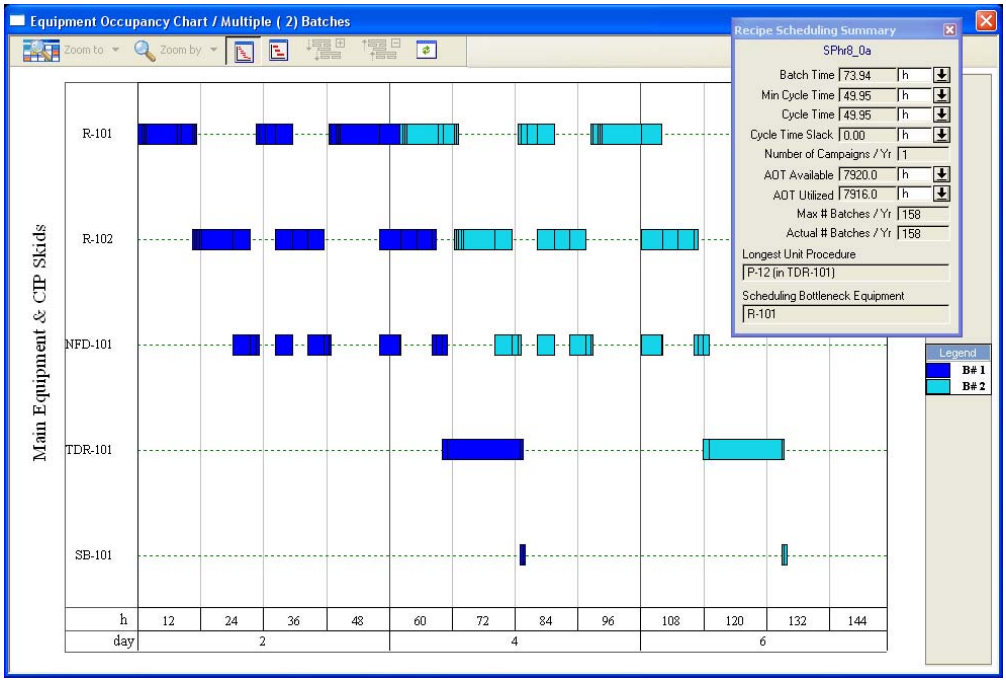


Figure 2.56: The Equipment Occupancy Chart for two consecutive batches.

The equipment with the least idle time between consecutive batches (or, equivalently, the longest occupancy time per batch) is the time (or scheduling) bottleneck ('R-101' in this case). This is the equipment that determines the maximum number of batches per year. Its occupancy time per batch (approximately 50 hours) corresponds to the minimum cycle time (the minimum possible time between consecutive batch starts). The actual recipe cycle time (the actual time between two consecutive batch starts) is equal to the minimum cycle time since the specified slack time between batches is zero for this example. The recipe batch time (the time required to complete a single batch) is roughly 74 hours.

SuperPro Designer also generates charts of resource demand as a function of time for raw materials, heating and cooling utilities, power, and labor. Figure 2.57 shows the 'Operator' labor resource demand (green line) for this example process and for 10 consecutive batches. A limit of 6 operators has been set through the chart's **Edit Style** menu and is also shown on the chart (red line). Note that for short periods of time there is a need for up to six operators. If this exceeds the actual number of operators available, then certain operations will need to be

delayed to accommodate the labor constraint. Inventory graphs for raw materials also can be generated in a similar way.

Figure 2.57: The 'Operator' labor resource demand chart for 10 consecutive batches.

For more details on the above charts, see 2.1k Viewing Scheduling, Equipment Utilization and Resource Tracking Results.

THROUGHPUT ANALYSIS AND DEBOTTLENECKING

SuperPro Designer is equipped with powerful throughput analysis and debottlenecking capabilities. These include the Utilization Factors chart and the Batch Size Potential chart.

Figure 2.58 shows the Utilization Factors chart for this example. This chart presents the capacity, time, and combined equipment utilization in each procedure. A batch size (throughput) bottleneck corresponding to the limiting procedure/equipment combination in terms of highest combined utilization ('P-10/R-102' in this case) is also indicated on the chart.

Furthermore, the Batch Size Potential chart for this example is shown in Figure 2.59. In this chart, the total flow of the 'Final Product' stream is used as reference for batch size (throughput) calculations. The chart shows for each procedure/equipment combination, the actual batch size (red dotted line) and three estimates (conservative, realistic, and theoretical) of batch size potential. For each estimation method, a size bottleneck is indicated on the chart. This corresponds to the procedure/equipment combination that has the smallest batch size potential based on that estimation method. For this example, the size bottleneck is 'P-10/R-102' using any of the above estimation methods.

For more details on these charts, see2.1l Throughput Analysis and Debottlenecking.

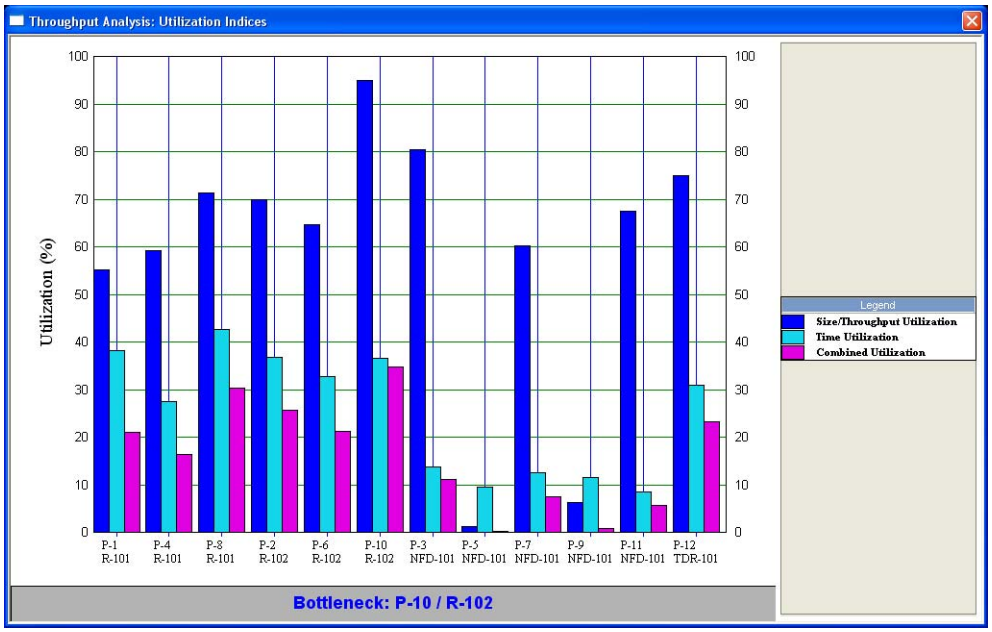


Figure 2.58: The Equipment Utilization Factors Chart.

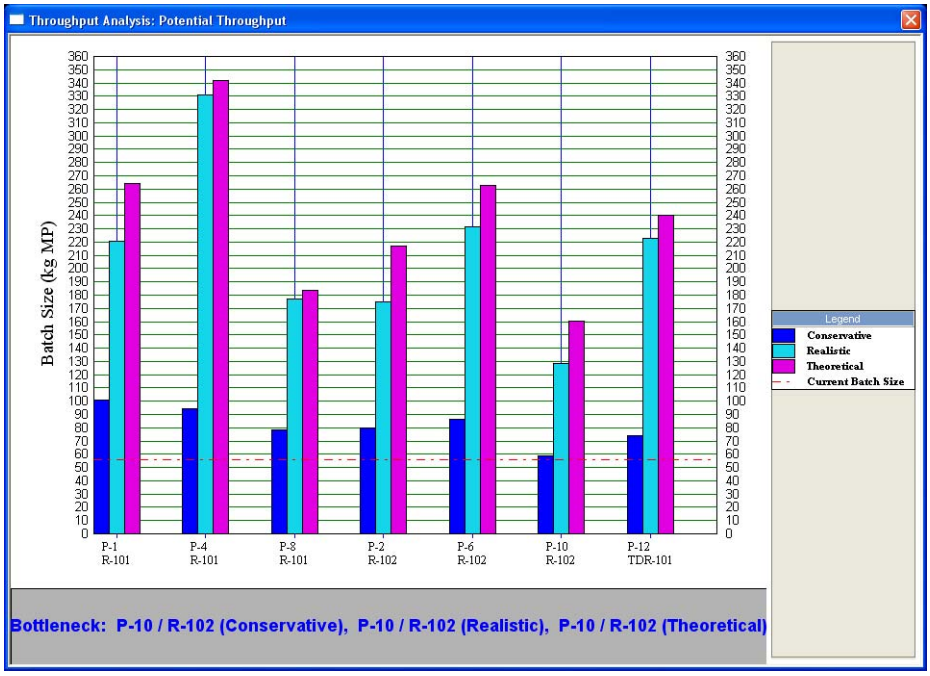


Figure 2.59: The Batch Size (Throughput) Potential Chart.

2.2f Cost Analysis and Economic Evaluation

SuperPro Designer performs thorough cost analysis and economic evaluation calculations and generates three pertinent reports. These are:

- the Economic Evaluation Report (EER),
- the Itemized Cost Report (ICR), and
- the Cash Flow Analysis Report (CFR).

Below are the key results of cost analysis for a plant producing 8,804 kg of this intermediate per year (around 55.7 kg per batch). The table shown in Figure 2.60 provides an overview of the total economic impact of the plant, including the total capital investment, annual revenues, and rate of return. This table was extracted from the PDF version of the Economic Evaluation Report (EER). To generate the EER, click **Economic Evaluation Report (EER)** on the **Reports** menu.

1. EXECUTIVE SUMMARY (2006 prices)

Total Capital Investment	9,503,000 $
Capital Investment Charged to This Project	9,503,000 $
Operating Cost	3,320,000 $/yr
Revenues	4,402,000 $/yr
Cost Basis Annual Rate	8,804.39 kg MP/yr
Unit Production Cost	377.10 $/kg MP
Unit Production Revenue	500.00 $/kg MP
Gross Margin	24.58 %
Return On Investment	15.75 %
Payback Time	6.35 years
IRR (After Taxes)	8.52 %
NPV (at 7.0% Interest)	865,000 $

MP = Total Flow of Stream 'Final Product'

Figure 2.60: The executive summary table of the Economic Evaluation Report (EER).

The table in Figure 2.61 provides a cost breakdown per cost item of the total annual operating cost over all process sections for this process. This table was extracted from the PDF version of the Itemized Cost Report (ICR). To generate the ICR, click **Itemized Cost Report (ICR)** on the **Reports** menu. The ICR enables the user to readily identify the cost-sensitive sections of a process – the economic hot-spots. For instance, Figure 2.61 reveals that the largest cost in this example is attributed to Facility-Dependent expenses that account for roughly 50% of the annual operating cost. An increase in equipment sharing may reduce this cost but may also reduce the annual throughput. Approximately another 17% of the annual operating cost is associated with raw materials. This is mainly attributed to the cost of quinaldine (a breakdown of overall material costs can be found in the EER). If a lower-priced quinaldine vendor could be found, the overall process cost would be reduced significantly. Labor and waste treatment/disposal costs are the third and fourth largest annual operating costs, respectively.

Labor can be reduced through increased automation. The environmental cost can be reduced through solvent recovery, purification, and reuse.

SUMMARY PER COST ITEM (Entire Process)

Cost Item	$/kg MP	$/batch	$/year	%
Raw Materials	64.260	3,581	565,766	17.04
Facility	189.169	10,541	1,665,520	50.16
Labor	83.932	4,677	738,970	22.26
Consumables	0.000	0	0	0.00
Lab/QC/QA	12.590	702	110,845	3.34
Utilities	0.009	0	78	0.00
Waste Trtmt/Disp	27.145	1,513	238,997	7.20
Transportation	0.000	0	0	0.00
Miscellaneous	0.000	0	0	0.00
TOTAL	377.105	21,014	3,320,177	100.00

Figure 2.61: The operating costs summary table of the Itemized Cost Report (ICR).

The above analysis shows how the economic reports can be used as a tool to optimize a process through 'what-if' scenarios by examining individual cost items:

- Would it make economic sense to use three reactors instead of two? It depends on how much the throughput would increase if three reactors were used, and how much the third reactor would add to the total cost.
- Would a radically modified purification scheme be better than the current scheme? It depends on what equipment, reagents, etc. would be required in the modified scheme, and what would be the impact on the overall product yield.

This type of what-if analysis is quickly and easily done using SuperPro Designer.

For a detailed 'what-if' analysis example, please refer to the Synpharm.doc readme file that can be found in the same directory as the SuperPro Designer files.

In addition, the CFR can be generated for this example by selecting **Cash Flow Analysis (CFR)** on the **Reports** menu. For more details on cost analysis and economic evaluation, see 2.1m Cost Analysis and Economic Evaluation.

2.2g Environmental Impact

You may also want to generate the Emissions Report (EMS) and the Environmental Impact Report (EIR) for this process. To do that, select **Emissions (EMS)** or **Environmental Impact (EIR)** on the **Reports** menu; for more details, see2.1n Environmental Impact.

2.3 THE B-GALACTOSIDASE PROCESS

This example analyzes the production of β-Galactosidase, an intracellular enzyme produced by *E.coli*. This example is recommended for users in the biotech and food industries. In addition, since this example is a batch process, it serves as a medium for discussing several scheduling issues.

The process file and readme files for this example can be found in the 'Examples\BGal' directory of SuperPro Designer. The following process files are included:

1. *Bgal8_0a*: This file represents the process at an early stage of plant design. All equipment is in 'Design Mode', meaning that all equipment sizes and throughputs are calculated as opposed to being specified by the user.
2. *Bgal8_0b*: This file represents the process after equipment sizes have been specified for key pieces of equipment.
3. *Bgal8_0c*: This file is the same the previous one, except that final product formulation and packaging unit procedures have been added.

For a detailed analysis of this example process using the above SuperPro Designer files, please refer to readme file 'Bgal.doc' that can be found in the same directory as the SuperPro Designer files.

2.3a Process Description

The β-Galactosidase (b-Gal) is an intracellular enzyme produced by *E.coli*. This enzyme has found limited industrial applications until now. It is mainly used in the utilization of cheese whey. More specifically, immobilized reactors with b-Gal have been developed to convert lactose found in cheese whey to glucose and galactose, yielding a sweetened product which can be used as an additive to ice cream, egg-nog, yogurt, and other dairy products. Another application of b-Gal is in the treatment of milk products. A significant number of people are lactose intolerant and cannot digest milk or milk products. Production of lactose-free milk products (using b-Gal reactors) allows those people to digest them.

The description that follows refers to file 'Bgal8_0b'. At this point, we suggest that you open this file and examine it briefly. We suggest that you keep the file open as you read the remainder of this section. This example analyzes a plant that produces 18,515 kg of b-Gal per year in 216 batches. This enzyme is normally produced by *E. coli* up to 1-2% of total cell protein under conditions of induction of the lac operon. Using genetic engineering, the level can go up to 20-25% of total protein. In this example, an easily attainable level of 10% is assumed.

The corresponding flowsheet for this process is shown in Figure 2.62. This process has been divided into three sections:

1. 'Fermentation' (black icons),
2. 'Primary Recovery' (blue icons), and
3. 'Purification' (green icons).

The concept of process sections was introduced to facilitate reporting of results for costing, economic evaluation, raw material requirements, and throughput analysis of integrated processes. A process section is a group of unit procedures that have something in common; for more details on process sections, see 2.2b Specifying Process Sections.

The process steps associated with each section of the example process are described below.

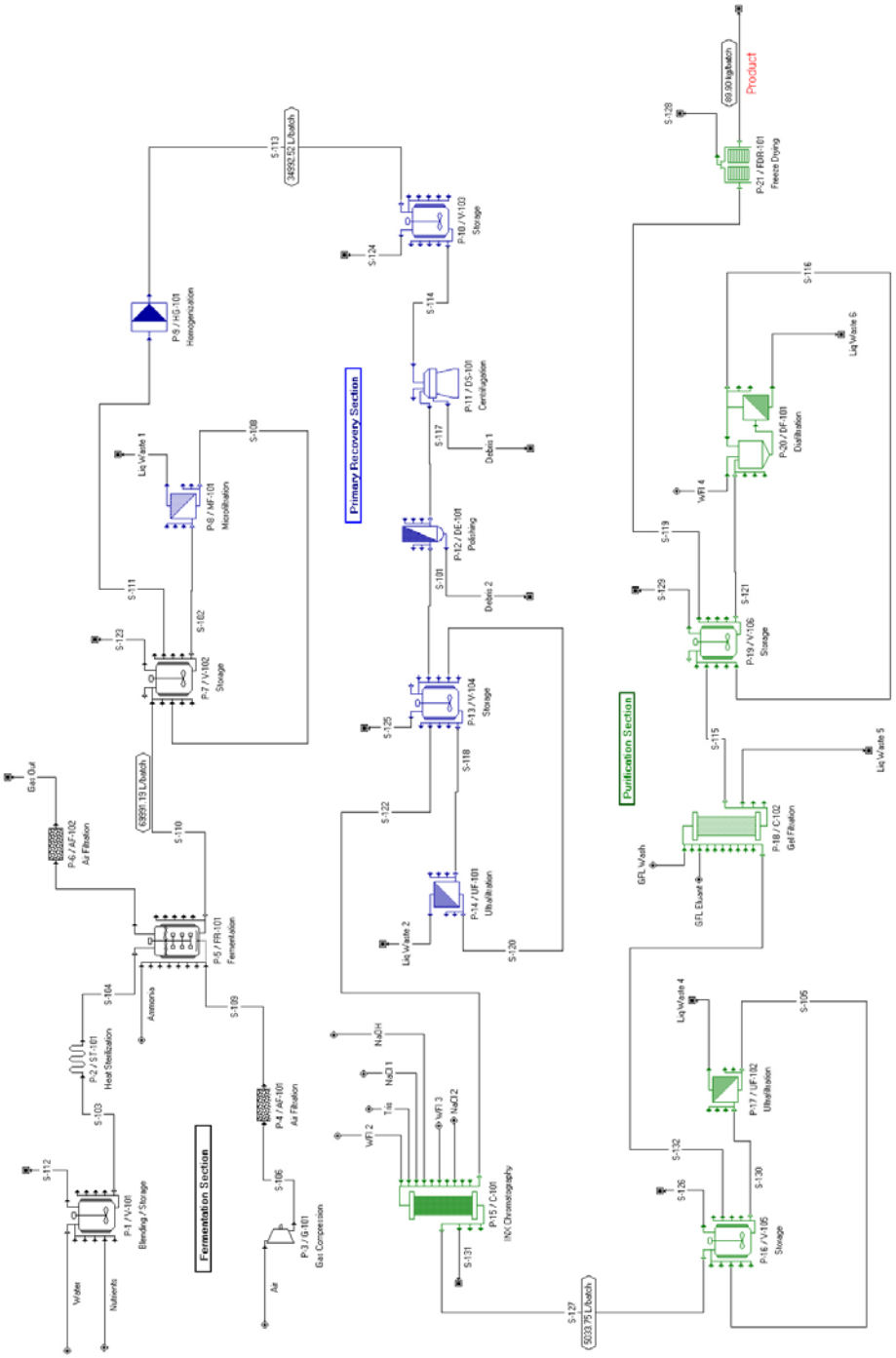


Figure 2.62: The β-Galactosidase process flowsheet.

FERMENTATION SECTION

Fermentation media are prepared in a stainless steel tank ('P-1/R-101') and sterilized in a continuous sterilizer ('P-2/ST-101'). A compressor ('P-3/G-101') and an absolute air filter ('P-4/AF-101') provide sterile air to the fermentor ('P-5/FR-101'). Gaseous ammonia is used as a nitrogen source for fermentation.

PRIMARY RECOVERY SECTION

The first step of the primary recovery section is cell harvesting to reduce the volume of the broth and remove extracellular impurities. It is carried out by a membrane microfilter ('P-8/MF-101'). Since b-Gal is an intracellular product, the next important step is cell disruption, performed in a high-pressure homogenizer ('P-9/HG-101'). After homogenization, a disk–stack centrifuge ('P-11/DS-101') is used to remove most of the cell debris particles. A dead-end polishing filter ('P-12/DE-101') removes the remaining cell debris particles. The resulting protein solution is concentrated two-fold by an ultra-filter ('P-14/UF-101'), and stored in a blending tank ('P-13/V-104').

PURIFICATION SECTION

Next, the product stream is purified by an ion exchange chromatography column ('P-15/C-101'). Then, it is concentrated three-fold by a second ultra-filtration step ('P-17/UF-102') and polished by a gel filtration column ('P-18/C-102'). Finally, a diafiltration unit ('P-20/DF-101') exchanges the gel filtration buffer, and the protein solution is lyophilized in a freeze dryer ('P-21/FDR-101').

2.3b Specifying Staggered Equipment

To cut the cycle time of a batch process, it is common to utilize multiple equipment items operating in staggered mode (i.e., alternating from batch-to-batch) for steps (procedures) that have long cycle times. That's the case with steps 'P-13/V-104', 'P-16/V-105' and 'P-19/V-106' of this process. Notice that a staggered equipment indicator ( ) is shown at the bottom left corner of the corresponding procedure icons to indicate that the above steps use staggered equipment. Those steps (involving storage tanks) have long cycle times because they receive material from previous steps and feed subsequent steps. If we employ two tanks for each of those steps that alternate from batch to batch, we can cut their cycle times in half. This is specified through the 'Stagger Mode' box that can be found in the 'Equipment' tab of a unit procedure's 'Equipment Data' dialog. This tab is shown in Figure 2.63 for step 'P-13/V-104'. If the number of units in a single set is "1", then specifying "1" or "2" extra set(s) of equipment units in stagger mode is equivalent to creating a pool of two or three equipment items that can alternate in use.

The impact of the use of staggered equipment can be visualized by looking at the Equipment Occupancy Chart (Figure 2.64) for this process. Tank 'V-104b' is the alternate of tank 'V-104' for step 'P-13'. The first batch (blue color) is handled by 'V-104', whereas the second batch (cyan color) is handled by 'V-104b'. The two tanks continue to alternate in subsequent batches. The same happens with tanks 'V-105' and 'V-105b' for step 'P-16', and tanks 'V-106' and 'V-106b' for step 'P-19'.

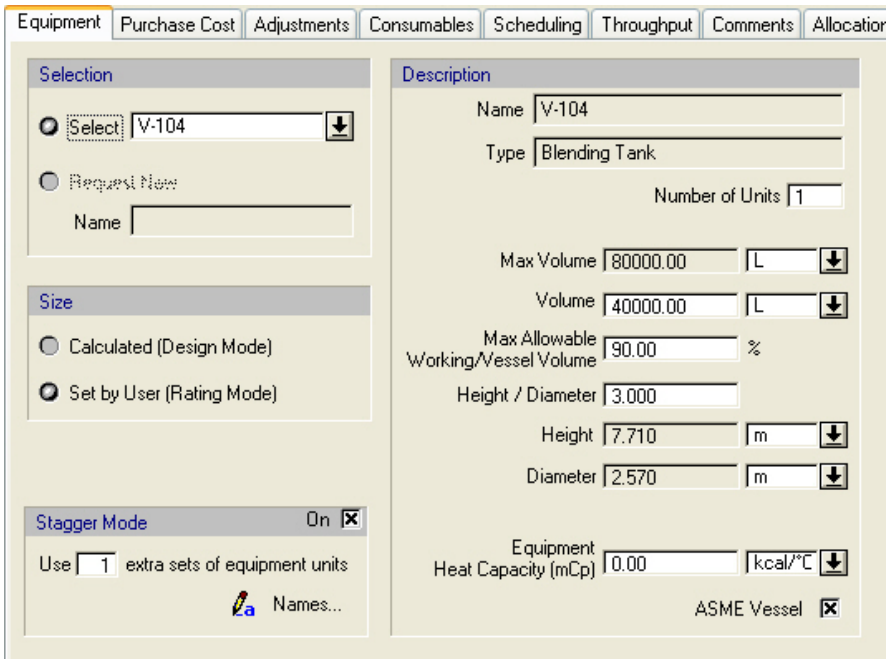


Figure 2.63: The Equipment tab of a storage vessel.

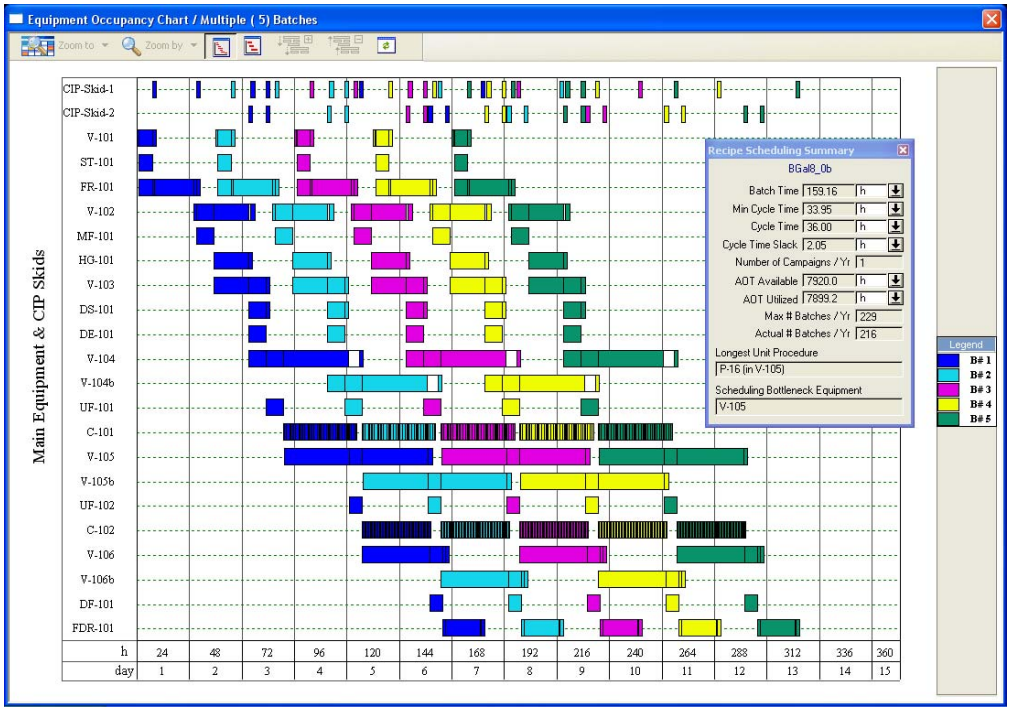


Figure 2.64: The Equipment Occupancy Chart for five consecutive batches.

The names of staggered equipment (e.g. 'V-104b') can be edited by clicking on the **Names** button in the 'Equipment' tab. For additional information on staggered equipment, see 6.1c Staggered Mode. For more details on the Equipment Occupancy Chart, see 2.1k Viewing Scheduling, Equipment Utilization and Resource Tracking Results.

2.3c Initializing Data Specific to Biotech Processes

PRIMARY BIOMASS COMPONENT, WATER COMPONENT AND EXTRA-CELL %

In bioprocessing, we have formation of intracellular (i.e., inside the cell) as well as extracellular (i.e., released into the solution) products. To capture this, as well as the fact that biomass is usually reported on a dry-cell-mass basis, we use the concept of 'Extra-Cell %' in streams and fermentation reactions. The 'Extra-Cell %' of a component in an input stream (something fed into the system) or a product of a fermentation reaction (something generated in the system) can be specified only if the 'Primary Biomass Component' of the process is identified. This is accomplished through the pure component registration dialog (see Figure 2.65). The 'Primary Biomass Component' is selected among components whose 'Is Biomass ?' flag has been set to true on the 'ID' tab of the corresponding 'Pure Component Properties' dialog; for more details on the pure component registration dialog, see 2.1e Registering Components and Mixtures.

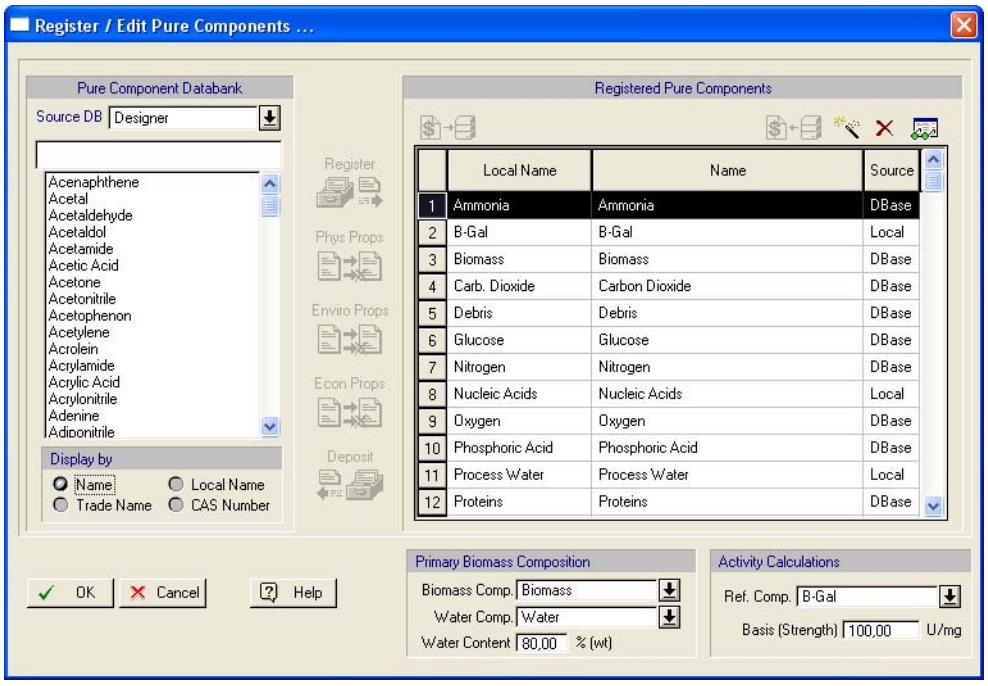


Figure 2.65: The pure component registration dialog for the b-Gal example.

In this dialog, you can also specify the water content of the 'Primary Biomass Component'. Here, water refers to the component that is selected as the 'Water Component' in the same dialog. If the primary biomass and water components are identified, and a positive value is specified for the water content of the primary biomass component, then, if there is formation of

the primary biomass component (as a fermentation product) in the process, the program will automatically associate intracellular water with biomass in order to satisfy its water content, as specified during component registration. In other words, the intracellular amount of the water component in the fermentation product stream will be set equal to the specified value for the water content of the primary biomass component. This is displayed using an 'Extra-Cell %' value of less than 100% for the water component in the 'Composition, etc.' tab of the simulation data dialog for the fermentation product stream (see Figure 2.66). This has an impact on material balances in separation procedures (e.g., centrifugation, clarification, filtration, etc.). If a removal percentage is assigned to the primary biomass component in these procedures, the program will use the same removal percentage for the intracellular portion of all components. This results in solids streams (e.g., retentate, concentrate, etc.) with concentrations closer to reality.

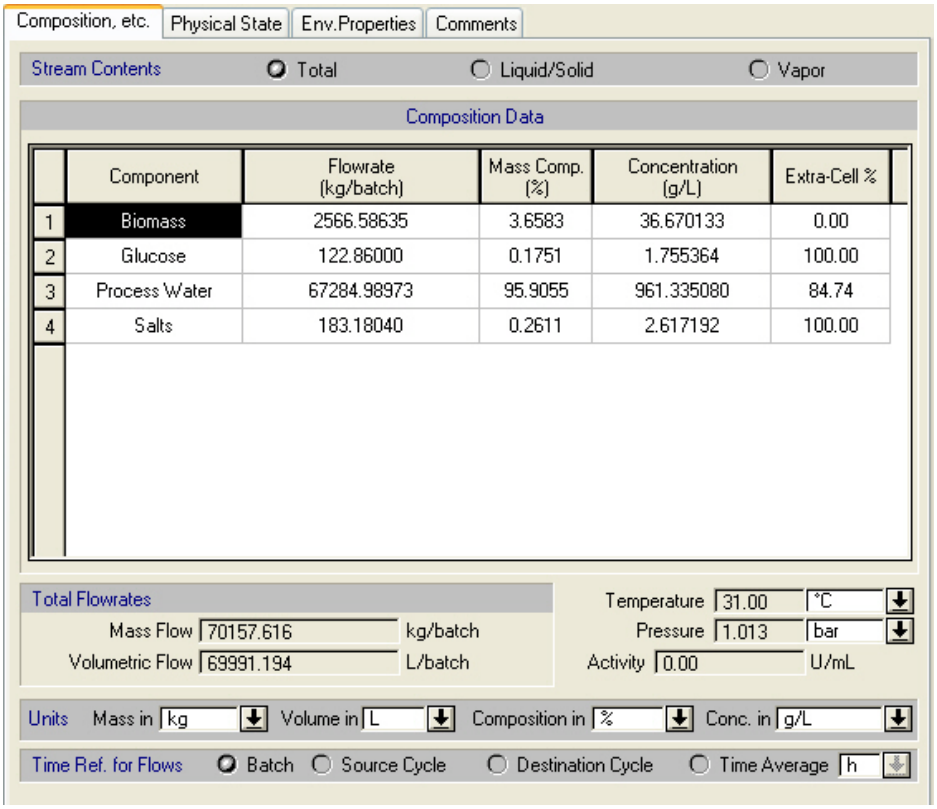


Figure 2.66: The 'Composition, etc.' tab of the simulation data dialog for fermentation outlet stream 'S-110'.

In addition, a fermentation reaction product can be identified as intracellular by specifying an 'Extra-Cell %' value of less than 100% in the 'Stoichiometry Balance for Reaction' dialog for that reaction. This dialog can be accessed through the 'Reactions' tab of a fermentation operation's dialog. That component can become extracellular (released into the solution) using a cell disruption procedure (e.g., high-pressure homogenization or bead milling).

ACTIVITY REFERENCE COMPONENT

In bioprocessing, the concentration of a product or undesired impurity is often reported as activity measured using a certain assay. In SuperPro Designer, this is represented using the 'Activity Reference Component' and its activity 'Basis' which is expressed in U/mg. These can be specified through the pure component registration dialog (see Figure 2.65). The activity basis represents how many (arbitrary) units of activity (U) correspond to each mg of the reference component present in a stream. This information is used to calculate and report the activity of a stream in U/mL. This concept is also applicable to other industries. For instance, in treatment of nuclear waste, the calculated stream activity may represent radioactivity.

INITIALIZING FERMENTATION OPERATIONS

Correct modeling of fermentation operations is important in biotech processes. SuperPro Designer is equipped with two different types of fermentation models (stoichiometric and kinetic) for batch, as well as continuous, fermentation reactions. The stoichiometric model is used if no kinetic data is available or if simplicity is desired, which is the case in this example. If kinetic data is available, the kinetic model can be used to calculate composition, temperature, and utility profiles as a function of time. Initialization of a stoichiometric fermentation is essentially identical to initialization of a stoichiometric chemical reaction, except that there is an option on the 'Oper. Cond's' tab for fermentor aeration; for more details on the initialization of stoichiometric chemical reactions, see 2.2d Initialization of Reaction Operations.

Note that all batch reactions have fed-batch capabilities and that a Perfusion fermentation operation is also available. For examples of kinetic, fermentation and fed-batch reaction models, please consult examples 'BKinRxn', 'BKinFerm' and 'FedBR', respectively. These can be found in the 'Examples\Misc' directory of SuperPro Designer.

2.3d Specifying Storage Units

As an alternative to adding explicit storage procedures to the process, you can specify implicit supply or receiving storage units which are not displayed graphically on the flowsheet. These units allow you to track material storage requirements in a process without further increasing its complexity. An example of using this feature is demonstrated in file 'Bgal8_0b'. In this file, two receiving units (a biowaste tank and an aqueous waste tank) are employed for collecting waste. For more details regarding storage units and their application in this example file, please refer to the readme file for the b-Gal example.

2.3e Process Analysis

At this point, you may want to change the values of certain parameters and redo the mass and energy balance calculations (click **Solve ME Balances** ( ) on the **Main** toolbar or on the **Tasks** menu, or simply hit **Ctrl+3** or **F9** on your keyboard).

You can view the calculated flowrate and composition of intermediate and output streams by visiting the simulation data dialog of each stream (double click on a stream, or right-click on a stream and select **Simulation Data**). Alternatively, you may use the 'Stream Summary Table' to view selected attributes (e.g., total flow, temperature and pressure) of selected streams. To show or hide the 'Stream Summary Table', click **Stream Summary Table** ( ) on the **Main** toolbar. Note that this table is empty when it is brought up the first time. To populate it, right-click on the table to bring up its context menu and select **Edit Contents**; for more details, see 2.2e Process Analysis.

In addition, you can generate the 'Streams & Material Balance (SR)' report. To do this, click **Streams & Mat. Balance (SR)** on the **Reports** menu. This report contains information on the overall process, raw material requirements, stream compositions and flowrates, as well as an overall material balance. Figure 2.67 shows the bulk materials table of the SR report for this process; for more details on this report, see 2.2e Process Analysis.

2.2 BULK MATERIALS (Entire Process)

Material	kg/yr	kg/batch	kg/kg MP
Process Water	16,723,431	77,423.292	911.365
Glucose	1,326,888	6,143.000	72.310
Salts	221,616	1,026.000	12.077
H3PO4 (5% w/w)	2,609,488	12,080.962	142.207
NaOH (0.5 M)	22,275,903	103,129.182	1,213.954
WFI	48,102,353	222,696.080	2,621.400
Air	10,219,698	47,313.418	556.936
Ammonia	85,320	395.000	4.650
NaCl (0.1 M)	29,774,876	137,846.648	1,622.620
NaCl (0.5 M)	2,524,995	11,689.791	137.603
Tris Buffer	35,299,940	163,425.647	1,923.716
TOTAL	169,164,508	783,169.019	9,218.838

Figure 2.67: The bulk material s table of the Streams & Material Balance (SR) report.

You may also want to generate the Emissions Report (EMS) and the Environmental Impact Report (EIR) for this process. To do that, select **Emissions (EMS)** or **Environmental Impact (EIR)** on the **Reports** menu; for more details, see 2.1n Environmental Impact.

For additional information on viewing simulation results, see 2.1i Simulating the Process and Viewing the Simulation Results.

SCHEDULING, EQUIPMENT UTILIZATION, AND RESOURCE DEMAND GRAPHS

SuperPro Designer generates the Operations Gantt Chart and the Equipment Gantt Chart that display scheduling and equipment utilization information, respectively, for single or multiple batches. From the Gantt chart interfaces, you can also modify the scheduling parameters of unit procedures, operations, equipment (in Equipment Gantt Charts only), as well as of the entire recipe, and immediately visualize the effects on the entire batch production. A portion of the Operations Gantt Chart for this example and for a single batch is shown in Figure 2.68.

Another way of visualizing the execution of a batch process as a function of time is through the Equipment Occupancy Chart. This chart shows in a graphical way how long each equipment is kept busy by some operation and how long it is just idle during batch processing. As described in 2.3b Specifying Staggered Equipment, this chart can also be used to visualize the impact of using staggered equipment. Figure 2.64 in that section displays the Equipment Occupancy Chart for five consecutive batches of this example process. Please generate this chart now. To view scheduling summary information for this process on the chart (as was done in Figure 2.64), right-click on the chart to bring up its context menu and check **Scheduling Summary**. You may also access or modify the recipe scheduling information by selecting **Edit Recipe Scheduling Info** on the same menu.

The equipment with the least idle time between consecutive batches (or, equivalently, the longest occupancy time per batch) is the time (or scheduling) bottleneck ('V-105' in this case). This is the equipment that determines the maximum number of batches per year. Its occupancy

time per batch (approximately 68 hours) would be the minimum cycle time (the minimum possible time between consecutive batch starts) if no staggered equipment were specified. However, in this example, we chose to operate the procedure with an extra piece of equipment ('V-105b') for 'V-105' in stagger mode. Having an extra piece of equipment in stagger mode reduces the minimum cycle time by a factor of two. Therefore, the minimum cycle time for this example is approximately 34 hours; for more details on staggered equipment and their effect on cycle time, see 2.3b Specifying Staggered Equipment. The actual recipe cycle time (the actual time between two consecutive batch starts) was set to 36 hours for this example (through the 'Recipe Scheduling Information' dialog). The recipe batch time (the time required to complete a single batch) is roughly 160 hours.

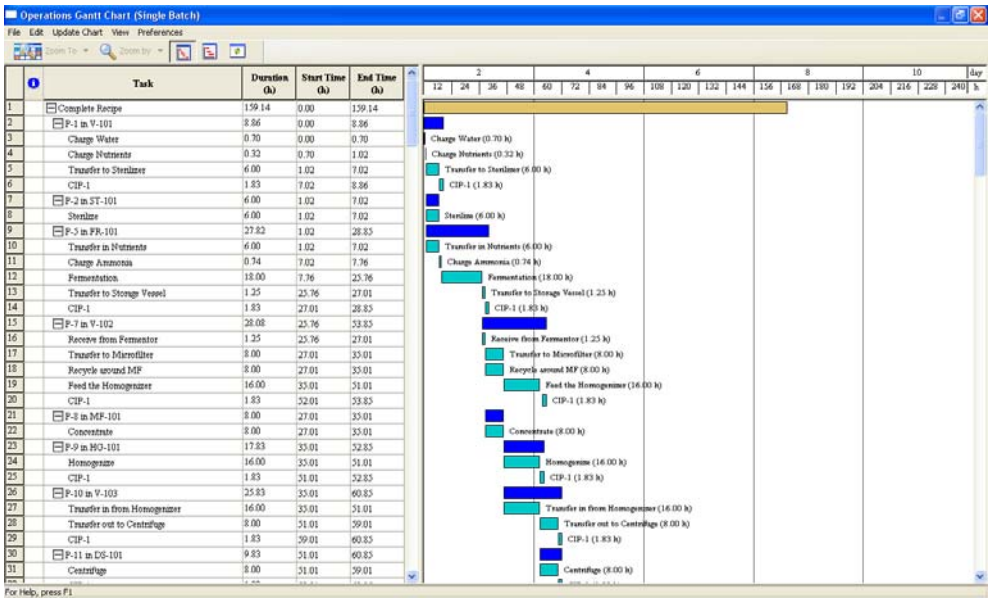

Operations Gantt Chart (Single Batch)
File Edit Update Chart View Preferences
Task
Duration (h)
Start Time (h)
End Time (h)
Complete Recipe 159.14 0.00 159.14
P-1 in V-101 8.86 0.00 8.86
Charge Water 0.70 0.00 0.70
Charge Nutrients 0.32 0.70 1.02
Transfer to Sterilizer 6.00 1.02 7.02
CIP-1 1.83 7.02 8.86
P-2 in ST-101 6.00 1.02 7.02
Sterilize 6.00 1.02 7.02
P-3 in FR-101 27.82 1.02 28.83
Transfer in Nutrients 6.00 1.02 7.02
Charge Ammonia 0.74 7.02 7.76
Fermentation 18.00 7.76 25.76
Transfer to Storage Vessel 1.25 25.76 27.01
CIP-1 1.83 27.01 28.83
P-7 in V-102 28.08 25.76 53.83
Receive from Fermentor 1.25 25.76 27.01
Transfer to Microfilter 8.00 27.01 35.01
Recycle around MF 8.00 27.01 35.01
Feed the Homogenizer 16.00 35.01 51.01
CIP-1 1.83 52.01 53.83
P-8 in MF-101 8.00 27.01 35.01
Concentrate 8.00 27.01 35.01
P-9 in HG-101 17.83 35.01 52.83
Homogenize 16.00 35.01 51.01
CIP-1 1.83 51.01 52.83
P-10 in V-103 25.83 35.01 60.83
Transfer in from Homogenizer 16.00 35.01 51.01
Transfer out to Centrifuge 8.00 51.01 59.01
CIP-1 1.83 59.01 60.83
P-11 in DS-101 9.83 51.01 60.83
Centrifuge 8.00 51.01 59.01
For Help, press F1

Figure 2.68: The Operations Gantt Chart for a single batch.

SuperPro Designer also generates charts of resource demand as a function of time for raw materials, heating and cooling utilities, power, and labor. Figure 2.69 displays the consumption of pure component 'WFI' (water for injection) for 5 consecutive batches of this process. To generate this chart, select **Materials ▸ Entering ▸ Multiple Batches** on the **Charts** menu. In the 'Ingredient Consumption Chart' dialog that appears, select pure component 'WFI'. Also, make sure that the options to include pure component participation in stock mixtures and discrete entities are not checked. This will ensure that the chart will display solely pure component consumption.

In this chart, the red line represents instantaneous consumption rate, the blue line represents time-averaged consumption rate (over a period of 12 hours) and the green line represents cumulative consumption amount (reset to zero every 12 hours). This information is specified through the 'Ingredient Consumption Chart Style' dialog. To open this dialog, right-click on the chart to bring up its context menu and select **Edit Style**. The chart provides useful information for sizing WFI systems:

- The tallest red peak (highest instantaneous demand) is useful information for sizing the pipe diameter of the circulation loop and its pumping capacity since the loop and the pump must be able to accommodate the highest instantaneous demand.
- The tallest green peak provides useful information for sizing the surge tank of the WFI system. It corresponds to the working volume of the surge tank if a 12-hour buffer capacity is required (i.e., a 12-hour supply even if the still is not operational during that period).
- The tallest blue peak provides useful information for sizing the still. The larger the averaging interval, the greater the size of the surge tank and the smaller the size of the still. In other words, there is a trade-off between still size and tank size in the sizing of WFI systems.

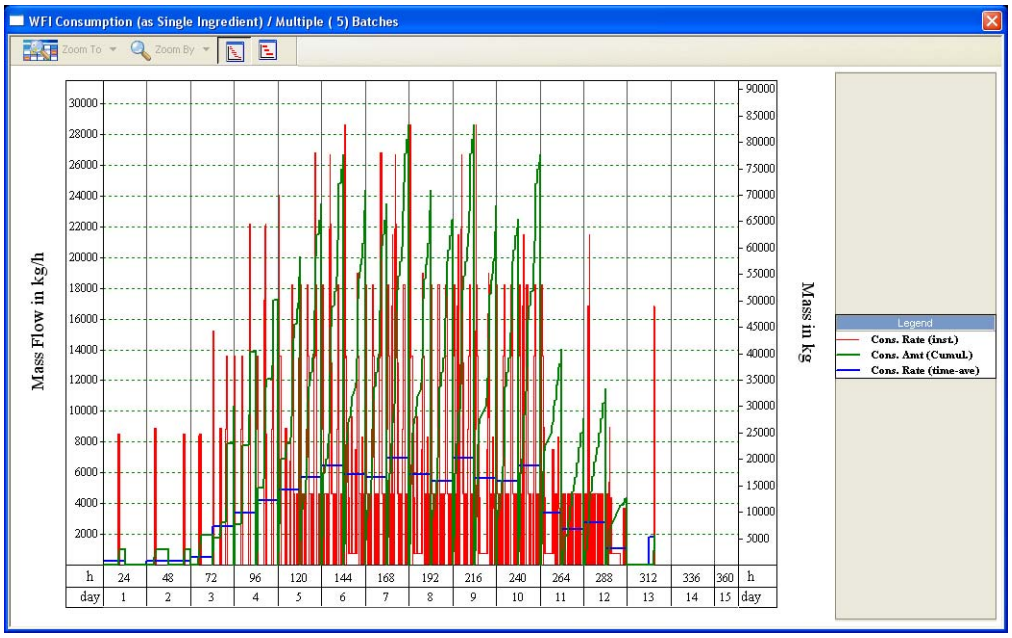

WFI Consumption (as Single Ingredient) / Multiple (5) Batches
Zoom To
Zoom By
Mass Flow in kg/h
Mass in kg
Legend
Cons. Rate (inst.)
Cons. Amt (Cumul.)
Cons. Rate (time-ave)
h 24 48 72 96 120 144 168 192 216 240 264 288 312 336 360 h
day 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 day

Figure 2.69: WFI Consumption Chart for 5 consecutive batches.

SuperPro Designer can also analyze and display inventory information for material resources. Suppose that there is a 100,000 kg WFI storage tank whose initial contents are zero. Suppose further that the WFI still has a rate of 20,000 kg/h and it is turned on when the level in the tank drops below 35% and off when it reaches 100%. The graph of Figure 2.70 shows the WFI level in the storage tank (green line) and the operation of the still (pink line) for five consecutive batches. To visualize the liquid level in the tank and the operation of the still, first select **Materials ▸ Entering, Inventory ▸ Multiple Batches** on the **Chart** menu. In the 'Ingredient Inventory Chart' dialog that appears, select pure component 'WFI' and make sure that the options to include pure component participation in stock mixtures and discrete entities are not checked (as was done for the WFI consumption chart). This will ensure that the chart will display solely pure component consumption. Then, click the **Supply Info** button to bring up the 'Resource Inventory Data' dialog for WFI. Specify the size of the tank, the rate of the still, the initial contents and the on/off criteria (the values provided above) and click **OK** to

return to the previous dialog. Then, click **OK** once more to close the 'Ingredient Inventory Chart' dialog and generate the chart.

For more details on the above charts, see 2.1k Viewing Scheduling, Equipment Utilization and Resource Tracking Results.

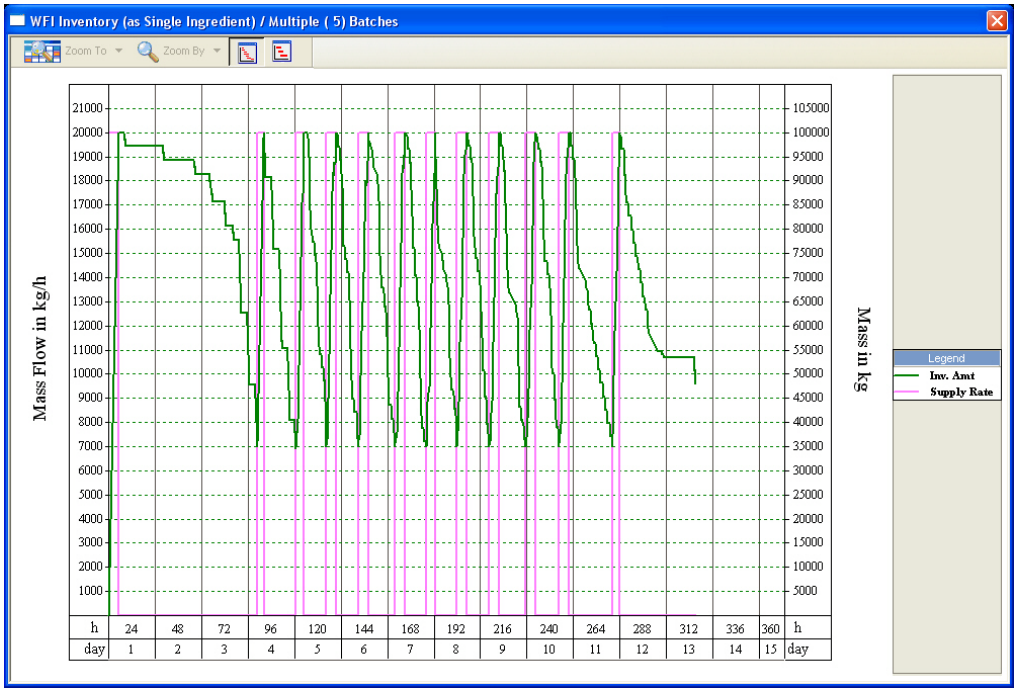


Figure 2.70: WFI inventory profile for five consecutive batches.

THROUGHPUT ANALYSIS AND DEBOTTLENECKING

SuperPro Designer is equipped with powerful throughput analysis and debottlenecking capabilities. These include the Utilization Factors chart and the Batch Size Potential chart.

Please generate the Utilization Factors chart for this example now. It can be seen that procedure 'P-15' that utilizes chromatography column 'C-101' has the highest combined equipment utilization. Therefore, that procedure/equipment combination is indicated on the chart as the size bottleneck in terms of combined utilization.

Next, please generate the Batch Size Potential chart for this example, using the flow of component 'B-Gal' in the 'Product' stream as reference. For this example, the procedure/equipment combinations 'P-18/C-102', 'P-7/V-102' and 'P-15/C-101' are based on conservative, realistic, and theoretical, estimates of batch size potential, respectively.

For more details on these charts, see 2.1l Throughput Analysis and Debottlenecking.

2.3f Cost Analysis and Economic Evaluation

SuperPro Designer performs thorough cost analysis and economic evaluation calculations and generates three pertinent reports. These are:

- the Economic Evaluation Report (EER),
- the Itemized Cost Report (ICR), and
- the Cash Flow Analysis Report (CFR).

Below are the key results of cost analysis for a plant producing approximately 18,350 kg of b-Gal per year. The table shown in Figure 2.71 provides an overview of the total economic impact of the plant, including the total capital investment, annual revenues, and rate of return. This table was extracted from the PDF version of the Economic Evaluation Report (EER). To generate the EER, click **Economic Evaluation Report (EER)** on the **Reports** menu.

1. EXECUTIVE SUMMARY (2006 prices)

Total Capital Investment	114,531,000 $
Capital Investment Charged to This Project	114,531,000 $
Operating Cost	110,242,000 $/yr
Revenues	183,293,000 $/yr
Cost Basis Annual Rate	18,514.49 kg MP/yr
Unit Production Cost	5,954.34 $/kg MP
Unit Production Revenue	9,900.00 $/kg MP
Gross Margin	39.86 %
Return On Investment	46.69 %
Payback Time	2.14 years
IRR (After Taxes)	34.61 %
NPV (at 7.0% Interest)	265,517,000 $

MP = Flow of Component 'B-Gal' in Stream 'Product'

Figure 2.71: The executive summary table of the Economic Evaluation Report (EER).

The tables in Figure 2.72 and Figure 2.73 provide cost breakdowns per cost item and per section, respectively, of the total annual operating cost over all process sections for this process. These tables were extracted from the PDF version of the Itemized Cost Report (ICR). To generate the ICR, click **Itemized Cost Report (ICR)** on the **Reports** menu. The ICR enables the user to readily identify the cost-sensitive sections of a process – the economic hot-spots. For instance, Figure 2.72 reveals that the cost of consumables is the largest cost in this example, accounting for roughly 53% of the total annual operating cost over all sections. This cost accounts for the expensive chromatography resins that need to be replaced periodically.

SUMMARY PER COST ITEM (Entire Process)

Cost Item	$/kg MP	$/batch	$/year	%
Raw Materials	1,040.704	89,204	19,268,101	17.48
Facility	1,022.509	87,645	18,931,241	17.17
Labor	577.133	49,469	10,685,319	9.69
Consumables	3,172.075	271,895	58,729,371	53.27
Lab/QC/QA	80.499	6,900	1,490,400	1.35
Utilities	21.889	1,876	405,269	0.37
Waste Trtmt/Disp	39.535	3,389	731,980	0.66
Transportation	0.000	0	0	0.00
Miscellaneous	0.000	0	0	0.00
TOTAL	5,954.344	510,378	110,241,681	100.00

Figure 2.72: The operating costs summary table per cost item of the Itemized Cost Report (ICR).

Furthermore, the table in Figure 2.73 reveals that the 'Purification' section is the most expensive part of this process. Thus, it would be wise to allocate resources to optimize this

section, as opposed to using those same resources elsewhere where optimization would have little effect on the overall project cost.

SUMMARY PER SECTION

Section	$/kg MP	$/batch	$/year	%
Fermentation Section	511.555	43,848	9,471,184	8.59
Primary Recovery Section	468.267	40,138	8,669,722	7.86
Purification Section	4,974.523	426,392	92,100,776	83.54
TOTAL	5,954.344	510,378	110,241,681	100.00

Figure 2.73: The operating costs summary table per section of the Itemized Cost Report (ICR).

The above analysis shows how the economic reports can be used as a tool to optimize a process through 'what-if' scenarios by examining individual cost items:

- Would it make economic sense to use a less expensive chromatography resin if it required more cycles to be run and more buffer solution to be used? It depends on how many more cycles are needed, and how much cheaper the new resin is.
- Would a radically modified purification scheme be better than the current scheme? It depends on what equipment, reagents, etc. would be required for the modified scheme, and and what would be the impact on the overall product yield.

This type of what-if analysis is quickly and easily done using SuperPro Designer.

In addition, the CFR can be generated for this example by selecting **Cash Flow Analysis (CFR)** on the **Reports** menu. For more details on cost analysis and economic evaluation, see 2.1m Cost Analysis and Economic Evaluation.

2.3g Environmental Impact

You may also want to generate the Emissions Report (EMS) and the Environmental Impact Report (EIR) for this process. To do that, select **Emissions (EMS)** or **Environmental Impact (EIR)** on the **Reports** menu; for more details, see 2.1n Environmental Impact.

2.3h Product Formulation and Packaging

SuperPro Designer contains a variety of formulation, packaging, and transportation unit procedures in order to capture the cost associated with such processes (see procedures 'P-21' to 'P-23' in file 'Bgal8_0c', for example).

Most material flows in SuperPro Designer are bulk material flows. Product formulation and packaging processes often involve formation and use of discrete entities, such as tablets, bottles, boxes, etc. The flow of such entities is represented by discrete streams, which are displayed by default in blue. Discrete procedures may be placed on the flowsheet and connected like any other procedure. Connection points for discrete streams are indicated by an open connection point, as shown in Figure 2.74 below.

To familiarize yourself with the formulation and packaging models and the concepts of discrete streams and entities, please open the 'Bgal8_0c' file that can be found in the 'Examples\BGal' directory of SuperPro Designer. Visit the simulation data dialogs of the various packaging unit procedures ('P-21' to 'P-23') and their corresponding operations and streams. Notice the different simulation data interface of discrete streams, which displays the flow of discrete

entities as well as the equivalent bulk flow (based on the bulk ingredients that compose the discrete entities). A discrete operation in these unit procedures may convert a bulk material stream into a discrete entity stream (e.g. bulk liquid product to filled bottles) or a discrete entity stream to another (e.g. unlabeled bottles to labeled bottles).

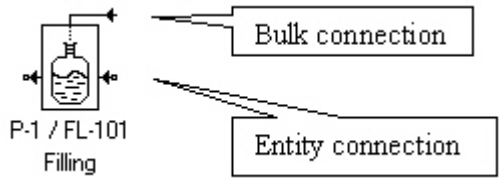


Figure 2.74: Stream connection points for bulk materials and discrete entities.

Another good example for dosage formulation and discrete processing can be found in the 'Examples\PhTablet' directory of SuperPro Designer. That example deals with a process that manufactures pharmaceutical tablets. For more information on discrete streams and entities, see Chapter 4 (Streams) or consult the Help documentation.

2.4 THE INDUSTRIAL WASTEWATER TREATMENT PROCESS

This example analyzes an industrial wastewater treatment plant and demonstrates how to track the fate of chemical components (constituents) in an integrated facility. It is based on file 'IWWT8_0' that can be found in the 'Examples\Indwater' directory of SuperPro Designer. This example is suitable for users with interest in biological wastewater treatment. Other relevant examples shipped with SuperPro Designer include 'MUNWATER', 'UPWATER' and 'GE'.

2.4a Process Description

This example represents a simplified version of an industrial activated sludge treatment plant. The corresponding flowsheet for this process is shown in Figure 2.75.

PROCESS SECTIONS

This process has been divided into two sections:

1. 'Bio-oxidation' (black icons), and
2. 'Sludge Treatment' (green icons).

The concept of process sections was introduced to facilitate reporting of results for costing, economic evaluation, raw material requirements, and throughput analysis of integrated processes. A process section is a group of unit procedures that have something in common; for more details on process sections, see 2.2b Specifying Process Sections.

The process steps associated with each section of the example process are described below.

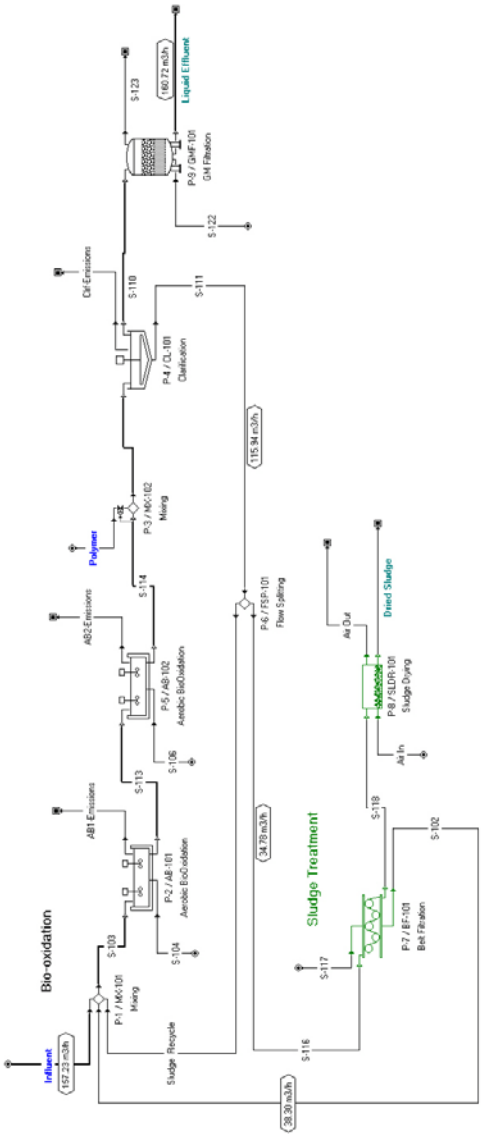


Figure 2.75: The process flowsheet of the example of biological treatment of industrial wastewater.

Bio-oxidation Section

The ‘Influent’ stream is combined with the ‘Sludge Recycle’ stream (‘P-1/MX-101’) and is sent to a sequence of two aeration basins (‘P-2/AB-101’ and ‘P-5/AB-102’) for biological oxidation of the organic material. Each aeration basin operates at an average hydraulic residence time of 6 hours and an average sludge residence time of 17-19 hours. A diffusion aeration system is used to maintain a minimum dissolved oxygen (DO) concentration of 2 g/L.

A clarifier ('P-4/CL-101') is used to remove the biomass and thicken it to around 10 g/L solids content. The liquid effluent from the clarifier is further treated using a granular media filter ('P-9/GMF-101') to remove any remaining particulate components.

Sludge Treatment Section

The withdrawn sludge stream ('S-116') is concentrated to a 15% wt. solids content using a belt filter press ('P-7/BF-101'). The removed water stream ('S-102'), which contains small amounts of biomass and dissolved solids, is sent back to the aeration basin. The concentrated sludge stream is dewatered to a final solids concentration of 35% wt. using a sludge dryer ('P-8/SLD-101').

At this point, please visit the interface dialogs of the various operations to check the specified parameter values. The bio-conversion reaction parameters are explained in detail later in this section.

CHEMICAL COMPONENTS

Please view the contents of the 'Influent' stream. The mass flowrate and composition of all pure components that are present in this stream are listed below:

Component	Flowrate (kg/h)	Mass Comp (%)
Benzene	100.00	0.0635
Biomass	15.66	0.0099
Glucose	783.00	0.4971
Heavy Metals	0.10	0.0001
Water	156,600.00	99.4294

This example corresponds to a relatively small plant with an average throughput of 1 million gallons per day (MGD). 'Glucose' represents the easily biodegradable components, while 'Benzene' represents the recalcitrant (not easily biodegradable) and volatile components. The 'Heavy Metals' component represents certain compounds that adsorb on biomass and follow its path in activated sludge plants.

Please visit the pure component registration dialog to view the physical and aqueous properties of the various components; for more details on this dialog, see 2.1e Registering Components and Mixtures. Some of the environmental properties of 'Glucose' are listed below:

Property	Value	Units
COD	1.066	g O/g
ThOD	1.066	g O/g
BODu / COD	0.732	g/g
BOD5 / BODu	0.9	g/g
TOC	0.4	g C/g
TP	0	g P/g

Property	Value	Units
TKN	0	g N (as NH_3)/g
NH_3	0	g N/g
NO_3-NO_2	0	g N (as NO_3,NO_2)/g

Values for such properties are available in the component database for many components. Whenever you enter a new component, you should visit its properties dialog to enter appropriate values for important properties. Note that these values, along with the stream compositions, are used to calculate the lumped environmental stream properties (BOD, COD, TKN, TSS, etc.); for more details on these properties, see Chapter 3 (Components and Mixtures).

STOICHIOMETRY AND KINETICS OF BIO-TRANSFORMATIONS

You can view the stoichiometry and kinetics of specified reactions in the two aerobic bio-oxidation operations (unit procedures 'P-2' and 'P-5') that are available in this example by visiting the 'Reactions' tab in the corresponding simulation data dialog for each operation. To edit the stoichiometry of a reaction, highlight that reaction in the 'Reaction Scheme' listing and click **Edit Stoichiometry** ( ). This will bring up the 'Stoichiometry Balance for Reaction' dialog. An example of that dialog can be seen in Figure 2.21. Similarly, to edit the kinetics of a selected reaction, click **View/Edit Kinetic Rate** ( ). This will bring up the 'Kinetics' dialog for the selected reaction. This dialog is shown in Figure 2.76 for the 'Glucose Degradation' reaction. As can be seen, the model offers great flexibility in specifying the kinetics of a bio-reaction. A bio-reaction operation (e.g., aerobic bio-oxidation) can handle any number of such reactions.

Make sure you look at the 'MUNWATER' example if you wish to distinguish between autotrophic and heterotrophic biomass and its impact on oxidation and nitrification / denitrification reactions.

The stoichiometry and kinetics of bioconversion reactions in this example are described below. The stoichiometry is on a mass basis.

Glucose degradation

$$\underset{1\ g}{\text{Glucose}} \rightarrow \underset{0.4\ g}{\text{Biomass}} + \underset{0.3\ g}{H_2O} + \underset{0.3\ g}{CO_2}$$

where:

- $kmax_0$ = 0.08 1/h at T = 20°C.
- theta = 1.04 (to account for the impact of temperature variations).
- K_s = 5 mg Glucose/ L.

For those of you who are used to thinking in terms of yield coefficients, the above stoichiometry is equivalent to a yield coefficient of 0.4 mg Biomass / mg Glucose.

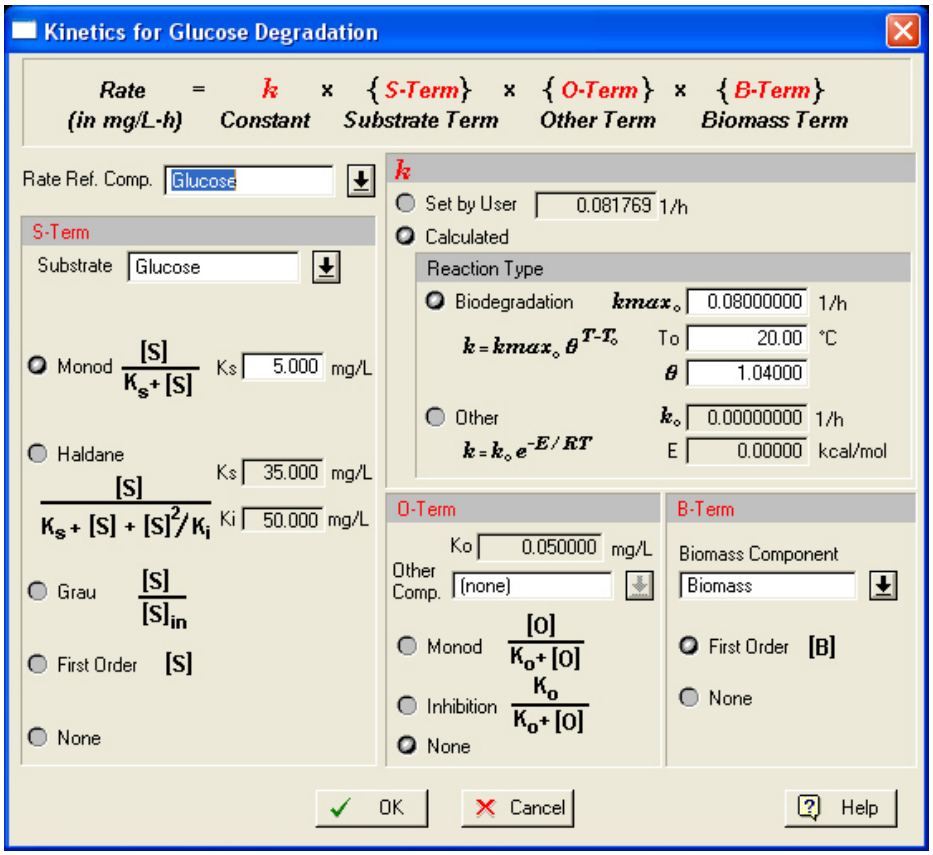


Figure 2.76: The Kinetics dialog of aerobic bio-oxidation reactions.

In SuperPro Designer, the user never specifies yield coefficients since that information can be extracted from the reaction stoichiometry.

In SuperPro Designer, we express the kinetic constants in terms of component concentration and not BOD5 because BOD5 is a stream property in SuperPro Designer and not a component. We treat BOD5 as a stream property and not as a component because many different components (e.g., Glucose, Benzene, etc.) may contribute to BOD5.

Benzene degradation - stoichiometry on a mass basis

$$\underset{1\ g}{\text{Benzene}} \rightarrow \underset{0.3\ g}{\text{Biomass}} + \underset{0.4\ g}{H_2O} + \underset{0.3\ g}{CO_2}$$

where:

- $kmax_0$ = 0.019 1/h at T = 20°C.
- theta = 1.04.
- K_s = 13.571 mg Benzene / L.

Biomass decay

Biomass → Dead Biomass
1 g 1 g

where k = 0.005 1/h.

In SuperPro Designer, biomass decay is handled through a separate reaction. In other words, you do not specify a decay coefficient but instead you specify a decay reaction with its own kinetic constants. This is a richer representation compared to the traditional way because it enables the user to distinguish between active and inert biomass.

In the above reactions we ignored the consumption of oxygen and nitrogen for the sake of simplicity. If you wish to consider it, simply modify the stoichiometry of the reactions and make sure that those components are available in the feed streams of the reactors.

VOC EMISSIONS

Volatile organic compounds (VOCs) in influent streams tend to volatilize from open tanks and end up in the atmosphere. Current US EPA regulations limit VOC emissions from treatment plants to no more than 25 tons per year (Van Durme, Capping Air Emissions from Wastewater, Pollution Engineering, pp. 66-71, Sept. 1993). SuperPro Designer can be used to predict VOC emissions using models that are accepted by the EPA. For a detailed description of the available models, please consult Chapter 10 (Emissions).

In this example, emissions occur from the two aeration basins and the clarifier. Please double-click on the emission streams to see the amount of benzene that is emitted. Around 12.3% of the total incoming benzene is emitted from the first aeration basin. A much smaller amount (around 0.13%) is emitted from the second aeration basin and essentially none is emitted from the clarifier.

SORPTION ON BIOMASS (SLUDGE)

In activated sludge plants, certain compounds (e.g., heavy metals) adsorb on biomass and follow its path. To account for that, you can specify the sorption percentage for each component that adsorbs on biomass through the 'Sorption' tab (see Figure 2.77) of the biological reaction operations. In this case, it was assumed that 90% of heavy metals adsorb on biomass.

For the sorption specifications to have an impact, you also need to identify the 'Primary Biomass Component' through the pure component registration dialog. If you use more than one biomass component (e.g., heterotrophic, autotrophic, etc. as in the 'MUNWATER' example), you should identify the heterotrophic bacteria (the most abundant) as your primary biomass; for more details, see 2.3c Initializing Data Specific to Biotech Processes. As described in that

section, the percentage of a component that is not associated with primary biomass in a stream is displayed on the stream dialog with the 'Extra-Cell %' variable.

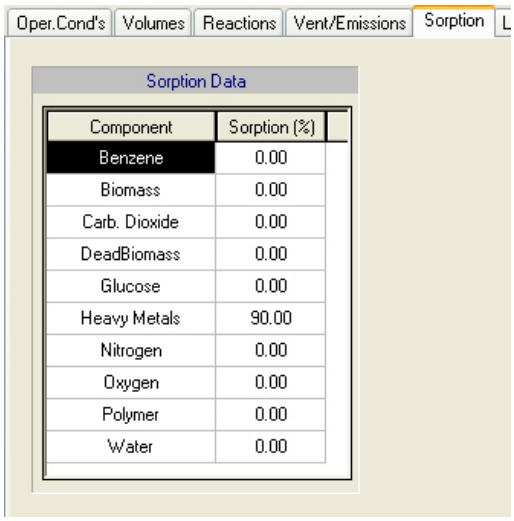


Figure 2.77: The Sorption tab of aerobic bio-oxidation operations.

Figure 2.78 shows the 'Composition, etc.' tab of the clarifier's sludge stream ('S-111'). In this

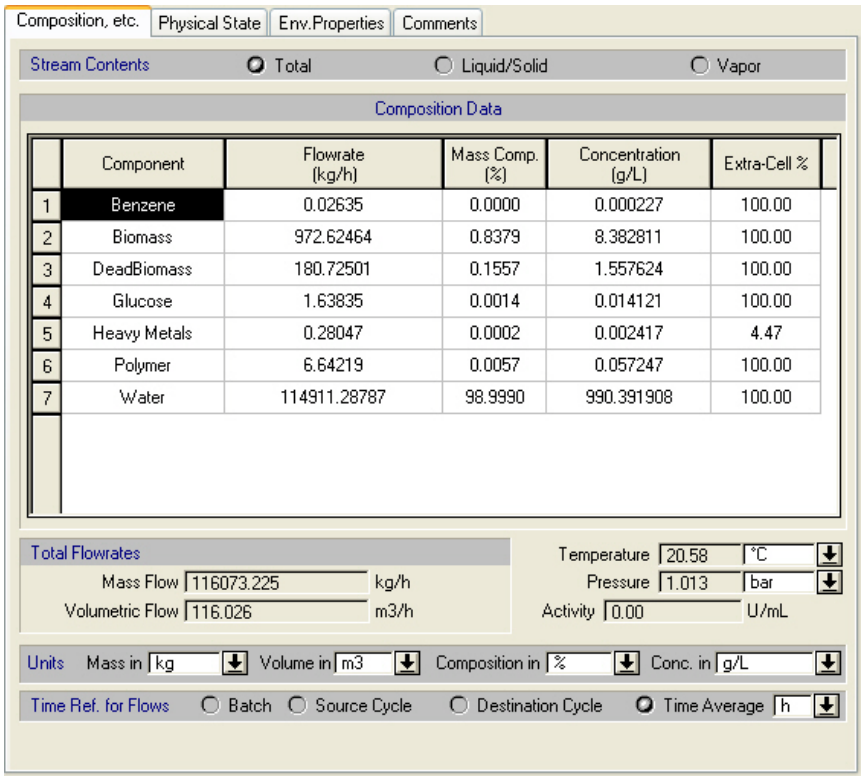


Figure 2.78: The 'Composition,etc.' tab of the sludge stream (S-111) of the clarifier.

case, 4.47% of the total amount of 'Heavy Metals' is extracellular (it remains in solution) and consequently 94.53% is associated with primary biomass. This information is utilized in the material balances of separation operations. For instance, if the removal percentage of the primary biomass in a clarifier is 99% (as is the case in this example), then 99% of an adsorbed component will follow the primary biomass component. Please visit the 'Liquid Effluent' and 'Dried Sludge' streams in the flowsheet to see how the 'Heavy Metals' are distributed between the two output streams (the vast majority end up in the 'Dried Sludge' stream).

2.4b Process Analysis

At this point, you may want to change the values of certain parameters and redo the mass and energy balance calculations (click **Solve ME Balances** ( ) on the **Main** toolbar or on the **Tasks** menu, or simply hit **Ctrl+3** or **F9** on your keyboard).

You can view the calculated flowrate and composition of intermediate and output streams by visiting the simulation data dialog of each stream (double click on a stream, or right-click on a stream and select **Simulation Data**). Alternatively, you may use the 'Stream Summary Table' to view selected attributes (e.g., total flow, temperature and pressure) of selected streams. To show or hide the 'Stream Summary Table', click **Stream Summary Table** ( ) on the **Main** toolbar. Note that this table is empty when it is brought up the first time. To populate it, right-click on the table to bring up its context menu and select **Edit Contents**; for more details, see 2.2e Process Analysis.

Clicking on the 'Env. Properties' tab of a stream's simulation data dialog will bring up the window shown in Figure 2.79. This dialog window displays the compositions and flowrates of the traditional environmental stream properties (e.g., BOD, COD, TOC, TSS, etc.). As described in 2.4a Process Description, the values of these properties are calculated based on the chemical composition of the stream and the contributions of the various stream components to these properties; for more details on these properties, see Chapter 3 (Components and Mixtures).

Information about water hardness expressed in $CaCO_3$ is used in water purification processes for sizing ion exchange columns and characterizing the purity of water. Please check the UpWater (ultrapure water) example for more details.

You may also want to have a look at the Environmental Impact Report (EIR), which contains information on the amount and type of waste that is generated by a manufacturing or waste treatment facility. The EIR also displays the compositions and flowrates of the traditional environmental stream properties (e.g., BOD, COD, TOC, TSS, etc.) for all the input and output streams of a process; for more details on environmental impact reports, see 2.1n Environmental Impact.

For more details on viewing simulation results, see 2.1i Simulating the Process and Viewing the Simulation Results

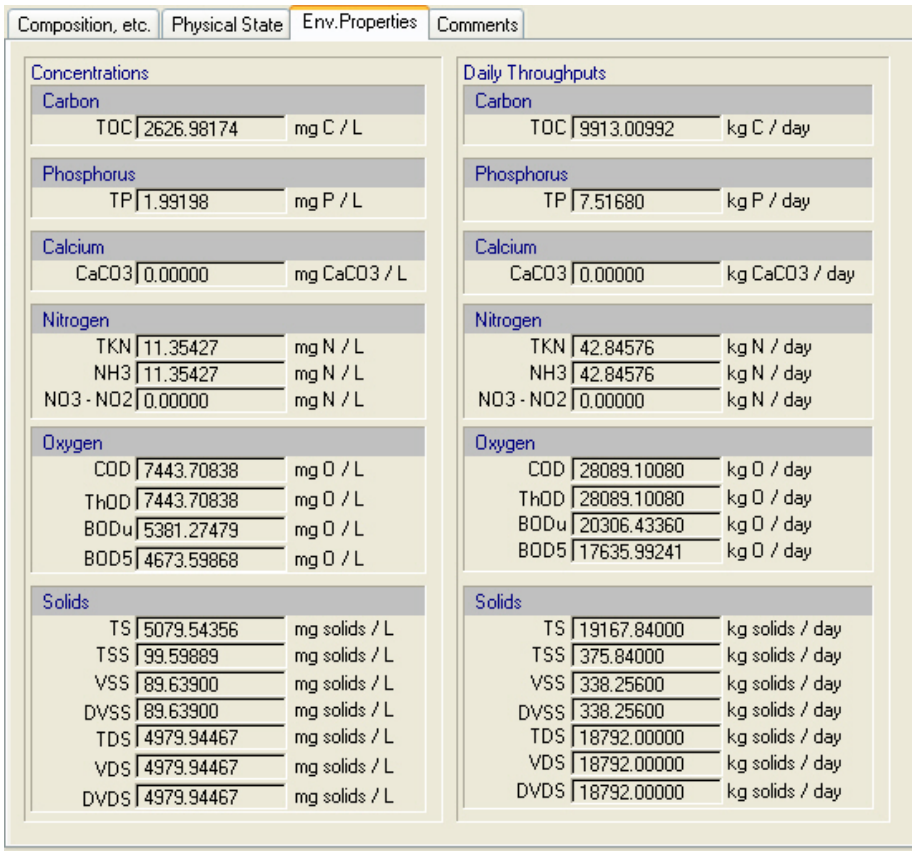

Composition, etc.
Physical State
Env.Properties
Comments
Concentrations
Carbon
TOC 2626.98174 mg C / L
Phosphorus
TP 1.99198 mg P / L
Calcium
CaCO3 0.00000 mg CaCO3 / L
Nitrogen
TKN 11.35427 mg N / L
NH3 11.35427 mg N / L
NO3 - NO2 0.00000 mg N / L
Oxygen
COD 7443.70838 mg O / L
ThOD 7443.70838 mg O / L
BODu 5381.27479 mg O / L
BOD5 4673.59868 mg O / L
Solids
TS 5079.54356 mg solids / L
TSS 99.59889 mg solids / L
VSS 89.63900 mg solids / L
DVSS 89.63900 mg solids / L
TDS 4979.94467 mg solids / L
VDS 4979.94467 mg solids / L
DVDS 4979.94467 mg solids / L
Daily Throughputs
Carbon
TOC 9913.00992 kg C / day
Phosphorus
TP 7.51680 kg P / day
Calcium
CaCO3 0.00000 kg CaCO3 / day
Nitrogen
TKN 42.84576 kg N / day
NH3 42.84576 kg N / day
NO3 - NO2 0.00000 kg N / day
Oxygen
COD 28089.10080 kg O / day
ThOD 28089.10080 kg O / day
BODu 20306.43360 kg O / day
BOD5 17635.99241 kg O / day
Solids
TS 19167.84000 kg solids / day
TSS 375.84000 kg solids / day
VSS 338.25600 kg solids / day
DVSS 338.25600 kg solids / day
TDS 18792.00000 kg solids / day
VDS 18792.00000 kg solids / day
DVDS 18792.00000 kg solids / day

Figure 2.79: Environmental and aqueous stream properties.

2.4c Cost Analysis and Economic Evaluation

SuperPro Designer performs thorough cost analysis and economic evaluation calculations and generates three pertinent reports. These are:

- the Economic Evaluation Report (EER),
- the Itemized Cost Report (ICR), and
- the Cash Flow Analysis Report (CFR).

Before looking at these reports, please visit the 'Stream Classification' dialog by selecting **Stream Classification** on the **Tasks** menu. The 'Influent' stream is classified as revenue and a unit processing cost of $8/MT (metric ton) is specified. In other words, we assume that this plant charges approximately $8/m^3 to the waste generators that use this facility to treat their wastewater. Please take a look at the unit treatment or disposal costs assigned to the various output streams. The dried sludge disposal cost is assumed to be $50/MT. Also, the disposal cost of aeration basin emissions is assumed to be $5/MT. Furthermore, the unit purchase prices of raw materials water and polymer are assumed to be $1/m^3 and $8.5/kg, respectively. Recall that

the price of a pure component or stock mixture is part of its properties, which can be edited when registering components; for more details, see 2.1e Registering Components and Mixtures.

Below are the key results of cost analysis for a relatively small plant with an average throughput of 1 million gallons per day (MGD). The table shown in Figure 2.80 gives an overview of the total economic impact of the plant, including the total capital investment, annual revenues, and rate of return. This table was extracted from the PDF version of the Economic Evaluation Report (EER). To generate the EER, click **Economic Evaluation Report (EER)** on the **Reports** menu. According to this table, if we had to build a plant of this size, the capital investment would be around $32 million (in year 2000 prices).

1. EXECUTIVE SUMMARY (2000 prices)

Total Capital Investment	32,028,000 $
Capital Investment Charged to This Project	32,028,000 $
Operating Cost	7,215,000 $/yr
Revenues	9,979,000 $/yr
Cost Basis Annual Rate	1,247,390,179.20 kg MP/yr
Unit Processing Cost	5.78 $/1000 kg MP
Unit Processing Revenue	8.00 $/1000 kg MP
Gross Margin	27.70 %
Return On Investment	14.19 %
Payback Time	7.05 years
IRR (After Taxes)	7.27 %
NPV (at 7.0% Interest)	612,000 $

MP = Total Flow of Stream 'Influent '

Figure 2.80: The executive summary table of the Economic Evaluation Report (EER).

The table in Figure 2.81 provides a cost breakdown per cost item of the total annual operating cost over all sections for this process. This table was extracted from the PDF version of the Itemized Cost Report (ICR). To generate the ICR, click **Itemized Cost Report (ICR)** on the **Reports** menu. The ICR enables the user to readily identify the cost-sensitive sections of a process – the economic hot-spots. For instance, Figure 2.81 reveals that the facility-dependent cost is the largest cost in this example, accounting for roughly 80% of the annual operating cost.

SUMMARY PER COST ITEM (Entire Process)

Cost Item	$/kg MP	$/day	$/year	%
Raw Materials	0.000	882	290,941	4.03
Facility	0.005	17,463	5,762,811	79.87
Labor	0.000	1,255	414,000	5.74
Consumables	0.000	0	0	0.00
Lab/QC/QA	0.000	188	62,100	0.86
Utilities	0.000	15	5,038	0.07
Waste Trtmt/Disp	0.001	2,060	679,926	9.42
Transportation	0.000	0	0	0.00
Miscellaneous	0.000	0	0	0.00
TOTAL	0.006	21,863	7,214,815	100.00

Figure 2.81: The operating costs summary table per cost item of the Itemized Cost Report (ICR).

The facility-dependent cost in this example is calculated for each section based on capital investment parameters. It accounts for maintenance, depreciation, and miscellaneous costs

(insurance, local taxes and other factory expenses). This information is specified through the 'Facility' tab of the 'Operating Cost Adjustments' dialog for each section. To open this dialog, select the appropriate section name in the 'Section Name' list box that is available on the **Section** toolbar and then click **Operating Cost Adjustments** ( ) on the same toolbar.

At this point, please visit the 'Facility' tab of the 'Operating Cost Adjustments' dialog for each section and uncheck the option named 'Include Depreciation' to ignore depreciation in the economic calculations. Depreciation can be ignored for very old plants or for plants that were built with public funding. Click **Perform Economic Calculations** ( ) on the **Main** toolbar to redo economic calculations. Then, please generate the ICR report. The table in Figure 2.82 shows the cost breakdown of the total annual operating cost over all sections when depreciation is not considered. It can be seen that the facility-dependent cost is the most important item even when depreciation is ignored.

SUMMARY PER COST ITEM (Entire Process)

Cost Item	$/kg MP	$/day	$/year	%
Raw Materials	0.000	882	290,941	6.72
Facility	0.002	8,717	2,876,461	66.45
Labor	0.000	1,255	414,000	9.56
Consumables	0.000	0	0	0.00
Lab/QC/QA	0.000	188	62,100	1.43
Utilities	0.000	15	5,038	0.12
Waste Trtmt/Disp	0.001	2,060	679,926	15.71
Transportation	0.000	0	0	0.00
Miscellaneous	0.000	0	0	0.00
TOTAL	0.003	13,117	4,328,465	100.00

Figure 2.82: The operating costs summary table per cost item of the Itemized Cost Report (ICR) when depreciation is ignored.

To estimate the labor cost, it is assumed that a total of 10,000 labor-hours (6,000 in the 'Bio-oxidation' section and 4,000 in the 'Sludge Treatment' section) are required to run the plant per year. This information is specified through the 'Labor' tab of the 'Operating Cost Adjustments' dialog for each section. Assuming that the plant can operate 330 days per year (this value is specified in the 'Plant Operating Mode' dialog, see 2.1c Specifying the Mode of Operation for the Entire Plant) and an operator can work for 6 labor-hours per day, then 5 operators (3 in the 'Bio-oxidation' section and 2 in the 'Sludge Treatment' section) are required to run the plant on a 24-hour basis. The basic labor cost rate is assumed to be $18/labor-hour. This cost is adjusted for a number of labor cost factors (benefits, supervision, etc.) resulting in an actual labor cost rate of $41.4/labor-hour. These factors are specified through the 'Properties' tab of the properties dialog for the 'Operator' labor resource. To access this dialog, right-click on the flowsheet to bring up its context menu and select **Resources ▸ Labor Types**. This will bring up the 'Labor Types Currently Used by the Process' dialog. Double-click on the 'Operator' labor type to display its properties dialog.

Note that several multipliers are used to estimate the capital investment of a treatment plant and perform its cost analysis and economic evaluation. Please read the first example of this chapter for more information on how to access and modify those multipliers. Many of the current default multipliers in SuperPro Designer are more appropriate for chemical manufacturing plants than for wastewater treatment plants. If you have better multipliers for wastewater treatment facilities, you may create a reference site in the 'Sites & Resources Databank' and deposit them there. This will allows you to use the specified multipliers in other process files by allocating your process sections to that site. For more information on how to take advantage of

the database capabilities of SuperPro Designer for cost analysis, please consult the 'SynPharmDB' readme file that can be found in the application's 'Examples\SynPharm' directory.

2.4d Modeling Challenges

This example can be used as a good starting point for modeling your own wastewater treatment plants. You may add more components and/or unit procedures to this process simulation in order to better approximate your own processes. For instance, you may add O_2, NH_3, and PO_4, and introduce appropriate reactions for tracking the consumption and generation of those compounds. The example on municipal wastewater treatment that can be found in the 'Examples\Munwater' directory of SuperPro Designer provides information on modeling of nitrogen removal.

As you increase the number of components, reactions, process steps, and recycle loops, SuperPro Designer will take longer to converge. For instance, reactions with very different reaction rates specified in a single unit procedure slow down the calculations considerably and may even cause convergence to fail. In such situations, it may be better to simplify your model by ignoring a slow reaction, at least at the early stages of analysis. For a fast reaction you may specify the stoichiometry and assume 100% conversion.

You are strongly advised to increase the complexity of your process simulation flowsheets in small steps so that you can be in a position to readily identify any changes that may potentially have slowed down the convergence or caused the simulation to fail.

2.5 ADDITIONAL INFORMATION

The use of SuperPro Designer, like most other software tools, requires a new way of thinking. This is particularly important for those of you who have little or no previous experience in process simulation. Remember that with simulation we only attempt to approximate the behavior of the real world. It is impossible to completely represent the behavior of a treatment plant on the computer. Consequently, your objective should be to limit the analysis to those variables that are of interest to you from a design (if the objective is to design a new plant or retrofit an existing one) or operations (if the goal is to improve the performance of an existing plant) point of view.

Please visit other examples (listed in the beginning of this chapter) for additional information regarding several SuperPro Designer features which may assist you in satisfying your modeling needs. For a detailed description of all software features, you may read through the rest of this manual or consult the Help documentation of the software. In addition, you may find answers to commonly asked questions in the Q&A file that is provided with the software.

If you have difficulty in using SuperPro Designer to its full potential, please do not hesitate to contact our technical support office. Our staff will be happy to assist you and provide you with guidance. Also, it may be a good idea to attend one of our training courses or arrange for a training course at your company's site. For more information, please visit our web site at intelligen.com.

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3 COMPONENTS AND MIXTURES

The material that is present during the physico-chemical transformations of your process is represented in SuperPro Designer by Pure Components and Stock Mixtures; entities that sometimes are collectively referred to as ingredients. Ingredients are primarily used to characterize (as amount and composition) the flow of all streams and equipment content of equipment with mass-holding capacity in a process simulation. Stock mixtures in particular are used mostly to expedite initialization of feed streams. They come very handy when certain raw materials (e.g., buffers) are always consumed by the process as a combination of pure components in a known composition. Sometimes ingredients are also consumed directly by an operation as special agents (without appearing on a stream). For example: a Gas-Sweep operation uses a material of choice as a sweeping agent; a CIP operation employs some material as cleaning agent, etc. There are many properties that describe each component (see 3.1e Pure Component Properties) and few that describe each mixture (see 3.2d Stock Mixture Properties). In order to facilitate the reuse of components and mixtures in several process simulations, SuperPro Designer comes equipped with two component and mixture databanks. The 'Designer' (or 'System') databank for components includes approximately 530 members. The 'Designer' databank for mixtures comes with over 40 entries. The 'Designer' portion of the databanks is maintained and occasionally updated by our staff. The 'User' segment of the databanks for components and mixtures is part of the 'User' database and allows for the user to create his/her own extensions of the 'Designer' database, by storing there his/her own pure components and stock mixtures according to their specific needs. SuperPro Designer also supports the 'DIPPR' pure component database in its relational database format (as developed and maintained at Brigham Young University). For more information on the component and mixture databanks, see 15.4 Pure Components Databank and 15.5 Databank of Stock Mixtures.

For users interested in modeling non-ideal mixtures and include rigorous vapor-liquid equilibria (VLE) models in their simulations, binary component coefficients are also required, see Vapor-Liquid Equilibrium Modeling. SuperPro Designer comes with a pair of databanks for binary coefficients as well (see 15.6 Binary Coefficients Databank).

In order to introduce a component or mixture into your process simulation, you must register it first (see 3.1a Pure Component Registration and 3.2a Stock Mixture Registration).

3.1 PURE COMPONENTS

A pure component (or sometimes mentioned simply as component) in a SuperPro Designer simulation represents the most elementary species that make up the composition of streams and vessel contents. Ultimately all mass and energy balances in SuperPro Designer are performed

at the component level. Examples of components are 'Water', 'Oxygen', 'Nitrogen', 'Biomass', etc. Please note that a pure component does not necessarily have to represent a single-molecule species. You may decide to use a pure component to represent 'Debris' in your process. Or, you may decide to use a pure component to represent 'Fats' in your process. That is acceptable, as long as you cannot expect the simulation to break such species into its constituents and as long as you provide for such components some reasonable values at least for their most commonly used properties (density, heat capacity, etc.). There may also be times when you may need to have two 'pure components' representing the same species but in different forms: for example, you may need two different pure components representing the same material in dissolved state and in crystal form. That is also acceptable (see info on page 3-4). Each pure component has a whole set of properties that describes its behavior (see 3.1e Pure Component Properties). You do not need to know precisely all of a component's property values in order to introduce it in your simulation as it is possible that the simulation models you have included in your process only need a limited set of component properties. Before you can engage a component in your process simulation you must register it (see 3.1a Pure Component Registration).

3.1a Pure Component Registration

Before you are able to use a material in your process as a pure component, you must define:

1. Its physical properties (molecular weight, density, heat capacity, critical properties, etc.)
2. A name tag by which this component will be known to the rest of the process elements (streams, operations, etc.). Since formal names (represented by the 'Name' property) tend to be very long, SuperPro Designer lets you define a shorter name tag (called the 'Local Name') for each component present in your process. Every component's 'Name' and 'Local Name' must be unique within your process.

After a pure component is registered, you can still edit its properties (see 'To edit the properties of a registered pure component...' on page 3-9). Note that the 'Name' cannot be edited; the 'Local Name' can be edited but not from the Pure Component Properties Dialog. You need to visit the Rename Pure Component Dialog to change the 'Local Name' of a pure component after it has been registered.

Instead of having to describe each component's properties from scratch, you can use one of SuperPro Designer's component databanks as a source to pull components into your process simulation (with their property values already defined); for more details, see 15.4 Pure Components Databank. If you cannot find the component that you need in the databanks you can introduce a new (your own) component. When starting a new process simulation, probably one of the first actions that you take is to introduce the components that will participate in the process. It is not necessary to provide an exhaustive list at the very beginning, because the members of the component-registry in a process file can be modified at any time. However, as good practice, it is recommended that as soon as you start a new simulation project, you should introduce (register) as many of the components that will be present as early as possible, as of most of the initialization parameters in streams and operations depend on the list of components present in the process (e.g., stream composition, component separation factors, key design components, etc.). If you add components after having initialized such operations, default values will be provided for the newly introduced components but you may be forced to revisit the i/o simulation dialog of the affected operations anyway.

To introduce (register) a component into your process, select the **Tasks ▸ Pure Components ▸ Register, Edit/View Properties** option from the main menu (or type **Ctrl+0** as a shortcut). Then, the Pure Component Registration Dialog appears. Components for a process can either be imported from the component databank or can be defined from scratch just for the needs of your specific simulation. When using the component databank as a source, component data will be pulled from one of the following database sources:

- The 'Designer' database
- The 'User' database
- The 'DIPPR' database
- The 'PPDS' database

For more details, see 15.4 Pure Components Databank.

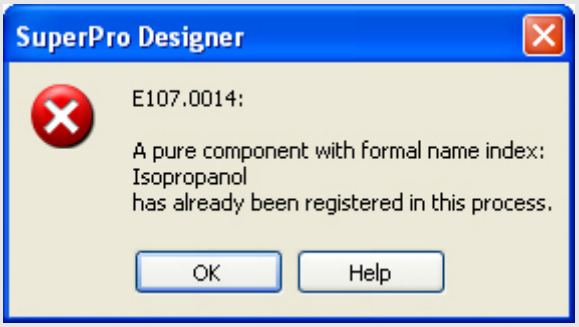
If you wish to pull a pure component from the databank, you must first choose the desired database source at the top left of the Pure Component Registration Dialog. Once you have selected a database as a source, the list box below will be filled with the contents of the selected database. The components in the databank are indexed and can be listed in one of four ways:

Component Indices (for 'Designer' & 'User' Databank)	Name (up to 31 char.) Trade Name (up to 31 char.) Chemical Abstract Service (CAS) Number (up to 15 char.) Local Name (up to 15 char.)
Component Indices (for 'DIPPR' Databank)	Name Chemical Abstract Service (CAS) Name Chemical Abstract Service (CAS) Number IUPAC Name
Component Indices (for 'PPDS' Databank)	Name Trade Name (Aspen Name in PPDS) Formula Chemical Abstract Service (CAS) Number

For some chemicals in the 'Designer' database, no CAS numbers could be found (or it didn't exist). Such chemicals are given made-up CAS numbers that are very easy to recognize: "N/A xxxx". The 'Local Name' is simply a shorter version of the full name of a chemical or it could represent a alias by which a chemical is known to the members of your organization. In any case, the 'Local Name' is the name by which a registered component will identify itself to the user in i/o simulation dialogs of operations and streams, reports, etc. and thus it becomes the

'ID-Tag' by which a component is known to the process. Therefore, the application will not allow you to register two components (or mixtures) with the same 'Local Name'.

Sometimes it is necessary to have the same chemical substance (e.g. NaCl) represent two different forms of that substance (e.g. in soluble form and as a crystal). After you have registered NaCl as a component for the first time (to represent the soluble form), you cannot re-register NaCl. If you did you would receive the following message:



To get around the fact that the application requires all registered components to have a unique (formal) 'Name' and 'Local Name', you should define a 'new' component on the New Component Definition Dialog with a 'Name' of "Sodium Chloride Crystals" using 'Sodium Chloride' as the starting component. Then, introduce that component into the process (using a different 'Local Name' - e.g. "NaCl-Cryst") and use it to represent the NaCl crystals.

In fact, the application will not allow you to register a component whose 'Local Name' or 'Name' clashes with any of the already registered components and mixtures. Note that the same restrictions apply when you attempt to register a stock mixture (see 3.2a Stock Mixture Registration). This restriction is necessary as commonly users have to choose an ingredient from either a component or a mixture list (e.g., when initializing the composition of an input stream). If two different ingredients were allowed to have the same name, or local name, then it would be impossible to know which one is selected.

Name conflicts are checked without regard to lower or upper case. In that sense, "Ethanol" will be considered the same name as "ETHANOL" or "ethanol". The reason is different sources (databases) of component information may include the same component with slightly different spelling (when it comes to letter case).

When copying-and-pasting parts of one simulation into another, all component-related information (e.g. retention factors in a filtration operation) are carried over. In order to make sure the infomation is carried over properly, the application will compare the component registry of the target (receiving) document, and if some components are missing, they will be automatically registered. Also, if some components are considered 'the same' they will be substituted by the ones pre-existing in the receiving document. In cases of components whose "Formal Name" or "Local Name" differs only up to letter case, then the actual spelling of the component (or mixture) as-is in the receiving document will be retained.

Sometimes you may need to register a component for the needs of your current simulation but you can't find it listed in any of the component databanks. At this point, you have two options:

(a) Introduce the new component in the user databank first (see 15.4b Adding and Deleting Pure Components); then pull it from the 'User' database into your process simulation using the Pure Component Registration Dialog. This may seem like a long, two-step procedure, but if you follow this approach, then the newly introduced component will

have a presence in the ‘User’ database, and it will always be readily available to be used for the needs of any future simulations.

(b) Introduce the new component directly in your process simulation from the Pure Component Registration Dialog. This option is useful if you don’t have good values for all the properties of the component at this time, or if you don’t think that any other future simulations may benefit from that component or if you simply don’t have any write-authorization to the ‘User’ database. Of course, if you change your mind later and decide to keep the component in the ‘User’ database, you can always do it from the same dialog .

The ‘Designer’ and ‘DIPPR’ databases contain equivalent data when it comes to estimating physical properties of pure components. However, the ‘Designer’ database also contains more data (economic properties & environmental properties) for each of its component record. The extra data are used when performing economic calculations and environmental assessments. Such data (purchase price, BOD, COD factors, etc.) are not available in the DIPPR database. If you imported a component originally from the ‘DIPPR’ or the ‘PPDS’ database, it will have default (mostly zero) values for all such properties. It is up to the user to edit those missing values (see ‘To edit the properties of a registered pure component...’ on page 3-9) or, if possible, to find the equivalent or similar component in the ‘Designer’ or ‘User’ database and copy its non-DIPPR data (see ‘To copy only a subset of component properties...’ on page 3-10.)

3.1b Pure Component Registration Dialog

This dialog appears when you select **Tasks ▸ Pure Components ▸ Register, Edit/View Properties** from the main menu of the application.

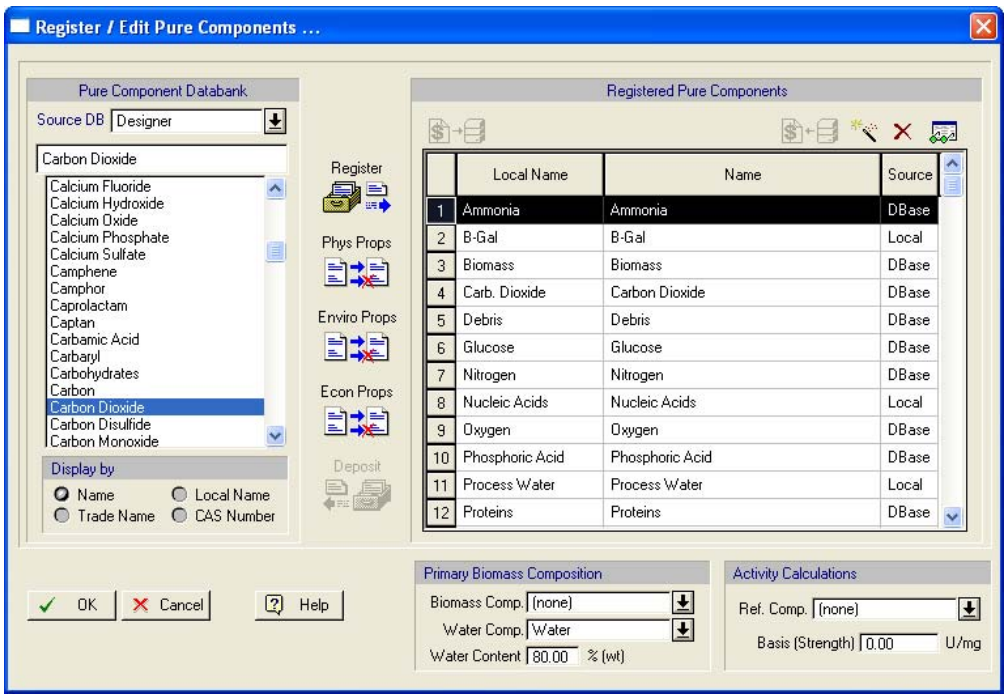


Figure 3.1: The component registration dialog.

Using this dialog you can:

- Introduce (add or register) a component into the process by importing it from a pure component databank.
- Introduce (add or register) an altogether new pure component (which does not exist in any of the pure component databanks).
- View and/or edit the properties of a registered component.
- Delete a component that is already registered in your process.
- Deposit a pure component already present (registered) in your process into the 'User' portion of your component databank. This is important if you have introduced a component directly into your process and later have decided to keep the component and its properties as part of your component databank for future reuse.
- Transfer (copy) physical, economic or environmental property data (as kept in the records of the 'Designer' or 'User' database) from a member of the component databank onto an already registered component that either lacks such data or has outdated data. This is especially useful when the registered component originated from the 'DIPPR' or 'PPDS' databases which lacks economic and environmental data.
- Reconcile (or synchronize) the property values of a registered pure component with its values in the databank (requires that the component has a databank record). You may decide to update the registered component's data using the databank record values or vice versa (update the databank property values from the values of the component in a process).
- Designate the 'special components' of 'Water' and 'Primary Biomass' (applies only to biochemical processes, see 3.1c Special Components.)
- Designate the 'Activity-Reference' component and specify the activity basis factor (see 3.1c Special Components).

▶ To register a pure component by importing it from the component databank...

1. Select the source database
   From the database selection list box, select the source database. Typically there are two options available to users: 'Designer' and 'User'. If you have purchased and installed 'DIPPR' (in its relational database format), then it will exist as the third choice. The 'PPDS' may also appear in the list if you have a licensed copy of the PPDS Thermodynamic Property Suite. As soon as you select a source database, its component contents will appear in the list box underneath.
2. Select a component from the available listing
   From the databank contents list box, select the chemical that you want to introduce in the process. If the 'Name' (or 'Local Name' or 'Trade Name' or 'CAS Number') is not visible, you may scroll up or down until you locate it, or start typing the first few characters of its name at the edit control above the list box. Notice that as you type the interface responds by automatically scrolling in order to bring the first entry that matches the typed portion of the

'Name' (or 'Local Name' or 'Trade Name' or 'CAS Number') at the top of the visible list. You may list the contents of the pure component databank by any of the available four indices: 'Name', 'Trade Name', 'CAS Number' or 'Local Name'.

3. Click on the **Register** button

As soon as you click on the **Register** button, the number of rows in the registration table shown on the right, will expand by one (the component order may change as components are listed alphabetically based on their 'Local Name').

4. You can repeat the above steps (1 through 3) to introduce more components. When you are finished introducing component, exit the Pure Component Registration Dialog with **OK**.

▶ To register a new component (not residing in the component databank) in your process simulation...

1. Click on the button
Fill in the fields of the New Component Definition Dialog that comes up. Even though only uniqueness of names within the process file will be enforced, it is recommended that you use unique strings across the whole 'User' database for the 'Name', 'Trade Name', 'CAS Number' and 'Local Name', in case you decide later to keep the component as a permanent member of the databank.

2. Specify a source component to be used for property value initialization
You must use another component as source for initializing the new component's property values. The source component can be part of the list already registered in your process or it can reside in a pure component databank.

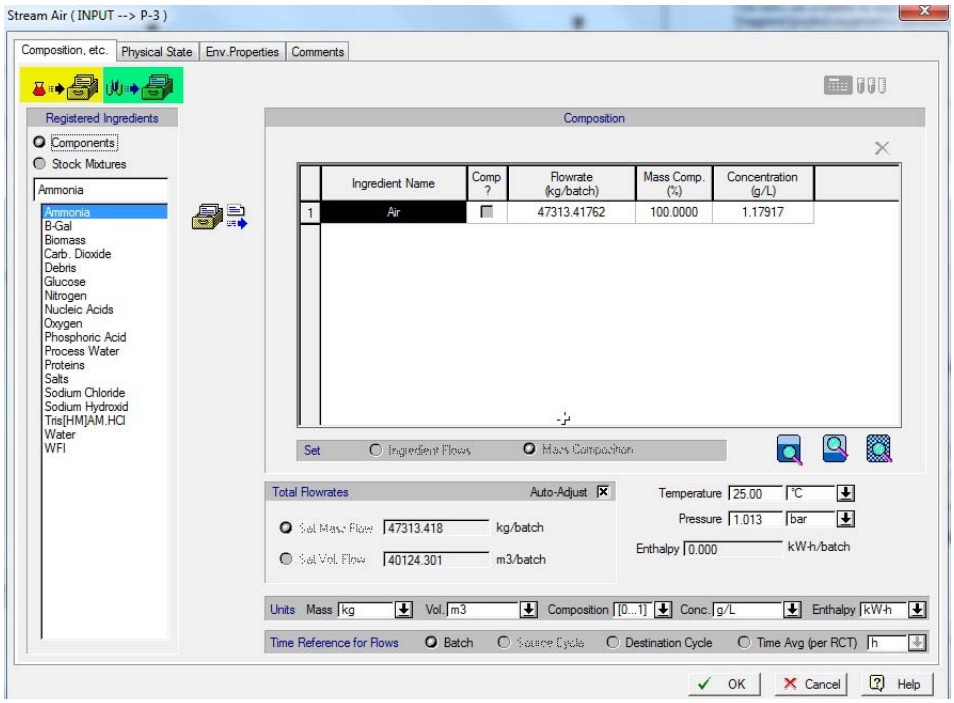
3. Click **OK**
Unless the program detects any conflicts in the name definitions, (all strings except the 'Formula' must be unique within the list of registered components) the new component will be added to the list of registered components.

4. If you need to introduce more components this way, repeat steps 1 through 3, and when you are finished adding components, exit the Pure Component Registration Dialog with **OK**.

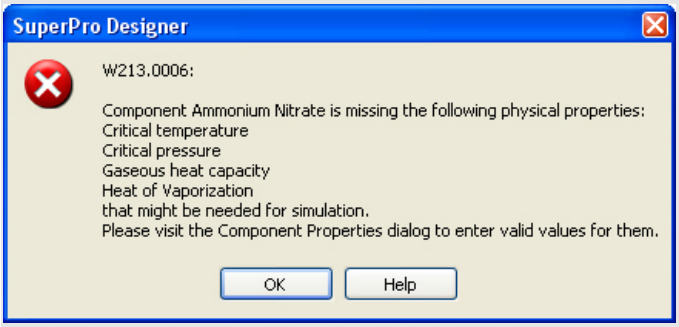
The list of registered components presented is alphabetical (based on the 'Local Name'). That is the same order that components are presented when one needs to choose say the "Design Component" in an operation, or to supply all component related information in operations (like, the "Rejection Coefficient" in an Ultrafiltration operation).

The presence of components is introduced in a process either through the initialization of a process input stream, or when a component appears to be the product of a reaction. To facilitate the introduction of a component (or a mixture) during the initialization of an input stream, users can click on the button (highlighted with yellow below) shown on the i/o input stream dialog (see below). The green highlighted button will bring up the Mixture Registration dialog (described elsewhere). After a new component (or mixture is added), it will become immediately available in the list of component ready to be included in the composition list of that input stream.

Clicking on the button shown above will invoke the same Component (or Mixture) Registration dialog mentioned previously,



In the 'Designer' component databank, few components don't have values for some of their properties. If you attempt to register such a component you will see the following message:



The application will still accept the registration of this component, but you must make sure that its missing property values are properly specified before this component is involved in the simulation of an operation whose model requires it. If you don't, then the operation's model will issue a warning when you attempt to execute the M&E balances.

You can modify any of the registered component's property values after it is register in your process (see 'To edit the properties of a registered pure component...' on page 3-9). The only exception is the component's 'Local Name' that cannot be modified from the component properties dialog (see below) but from the Rename Pure Component Dialog (select **Tasks ▸ Pure Components ▸ Rename** *from the application's main menu).*

▶ To edit the properties of a registered pure component...

1. Select the component in the registration table
   Locate the component in the registration table and click on the row that represents the component. Notice that when you click on it, the whole row is highlighted.
2. Click on the button.
   The Pure Component Properties dialog appears with all the properties of the selected component ready to be viewed and/or edited.
3. To keep the changes you made on the selected component's properties, exit the Pure Component Properties Dialog by clicking on **OK**. The changes are still not permanent. They will become permanent when you exit the Pure Component Registration Dialog by clicking **OK**. If you don't exit the Pure Component Registration Dialog with **OK** but by clicking **Cancel**, any component property modifications you made will be lost.

Modifying the properties of a registered component that was pulled from a component databank does not affect the property values of the original component record in the databank. It will also not affect the component properties of the same component used in simulations by others sharing the same component databank(s) with you.

▶ To delete a registered pure component...

1. Select the component in the registration table
   Locate the component in the registration table and click on the row that represents the component. Notice that when you click on it, the whole row is highlighted.
2. Click on the **Delete** the button.

▶ To deposit a registered pure component into the databank...

1. Select the component in the registration table
   Locate the component in the registration table, and click on the row that represent the component. Notice that when you click on it, the whole row is highlighted.
2. Make sure that 'User' is displayed at the top left listbox as the 'Source Database'.
3. Click on the **Deposit** button

If the component does not exist in the 'User' database currently, it will be added. If the component already exists in the database, the program will request a further confirmation that indeed the intention is to update the existing component's properties in the databank. In

any future project that you may need to import that component from the databank, the component will have the newly assigned set of values.

Please remember that any changes in the 'User' database as a result of any action on this dialog will be permanent and will not be reverted even if you exit the Pure Component Registration Dialog with ***Cancel****.*

Sometimes you may need to copy only a subset of properties from one component onto another. This situation will often arise when you have registered a component that was originally pulled from the 'DIPPR' or 'PPDS' databases. Since these databases not keep the full set of a SuperPro Designer component properties (e.g. purchase price, BOD content, COD content, etc.), when such a component is originally registered, by default, all these properties are initialized to zero. You could visit the Pure Component Properties dialog and edit those values yourself. SuperPro Designer offers you another choice. If you find the same (or a similar) component in the 'Designer' or 'User' database, you can copy all the non-physical property values from that component with just a click of button (see below).

▶ To copy only a subset of component properties...

1. Select the target component in the registration table.
   Locate the component in the registration table, and click on the row that represent the component. Notice that when you click on it, the whole row is highlighted.
2. Select a component database.
   Select one of the available component databases to display its contents.
3. Select the source component.
   From the contents of the selected database, select the component you wish to use as the source of the component properties.
4. Click on **Phys Props**, **Enviro Props** or **Econ Props** button
   Depending on the button you chose, the corresponding set of properties will be copied from the source component (in the databank) onto the target component (in your process file). Notice that the **Enviro Prop** and **Econ Prop** buttons are not available if the source component resides in the 'DIPPR' or 'PPDS' database because this repository of property data does not include such properties.

▶ To synchronize the economic properties of a registered pure component with its 'User' database record...

1. Select a registered pure component which currently exists in the 'User' portion of the databank. In order for a component to be verified as 'existing' in the 'User' database, its 'Name' must match exactly with one of the records in that database.
2. Click on the button to update the economic properties of the registered pure component from the record in the 'User' database.
3. Click on the button to update the economic properties of the component record in the 'User' database based on the current values of the registered component. Please remember that any changes in the 'User' database as a result of this action will be permanent and will not be reverted even if you exit the registration dialog with **Cancel**.

3.1c Special Components

Certain components in the set of registered components in a process file have a special meaning for the application's simulation engine. These components are selected from the Pure Component Registration Dialog. Currently, there are three such components:

1. The 'Primary Biomass' component:
   The component assumed to represent the biomass in the current process (recipe). Portions of other components that are considered intracellular (or sorbed) will be assumed to be incorporated into the mass (amount) of this compound and follow the fate of this component when separated from the main process stream (e.g. through a filter). If the component designated as 'Primary Biomass' is formed (as a reaction product) and the 'Water' component has been identified (see above definition) the application will adjust automatically the intracellular water in order to satisfy the biomass water content as specified on the Pure Component Registration Dialog. If the 'Primary Biomass' component has been assigned a removal coefficient, the system will use the same removal coefficient for components that have an intracellular portion. The 'Primary Biomass' component is selected only amongst component whose 'IsBiomass' flag has been set (see 'Pure Component: IDs' on page 3-13).
2. The 'Water' component:
   The component designated to represent the liquid form of water that makes up a large percentage of the biomass.
3. The 'Activity-Reference' component:
   If a component has been designated as the 'Activity-Reference' component then its concentration, along with the potency index or basis (also defined on the Pure Component Registration Dialog), is used to determine the activity strength of a stream. The potency index of a component represents how many (arbitrary) units of activity (U) should be accounted for each mg of the active component present in a stream. The activity value of a stream is displayed on the first tab of a stream's i/o simulation dialog.

Some unit operation models may treat a component (e.g. the component representing 'Oxygen' or 'Nitrogen' in your process) in a unique way. If that is this case, the identification of such components is done at that particular operation's i/o dialog and the scope of such identification is restricted within that operation model only.

3.1d Pre-Registered Components

As soon as a new project is started, SuperPro Designer will automatically introduce (register) from the 'Designer' databank into your process file three components:

- 'Water'
- 'Oxygen'
- 'Nitrogen'

'Water' is introduced as it is the most commonly used component in all process simulations. 'Oxygen' and 'Nitrogen' are also commonly used, and they are needed to be registered in order for the application to be able to automatically register, 'Air' as a stock mixture (see 3.2c Pre-

Registered Mixtures). You cannot delete (from the Pure Component Registration Dialog) the pre-registered components (or mixtures).

3.1e Pure Component Properties

Each component is identified in a process by its 'Local Name', which is a user-defined identification tag. A component's 'Local Name' can be up to 15 characters long and it is used instead of the component's (typically long) 'Name' (or 'Formal Name') in composition tables of i/o dialogs of streams, separation tables of i/o operation dialogs, reports, etc.

In order to carry out the material and energy (M&E) balances, the program needs to know the fundamental properties of each component (such as molecular weight, liquid/solid density, normal boiling point, critical temperature, critical pressure, compressibility factor, Henry's constant, Antoine constants, etc.). These properties are called **fundamental properties** because all other properties (**derived properties**) are calculated based on the values of these properties. The fundamental properties are listed below. You should make every effort to provide the program with as accurate values of fundamental component properties as possible as it is very likely that their values will affect the accuracy of the simulation results.

A component's property may be used only in certain unit operation models. You only need to provide accurate values for component properties that are used by the models included in your process simulation. The input data report (component section) mentions for each component's property if it is used or not by the current models when the M&E balances are executed.

Oftentimes users provide accurate values only for the minimum properties required for the current state of their process simulation and later, as the process model is extended or modified and more procedures and operations are included, they neglect to revisit the component property dialogs and update the component properties. As each new component introduced in the process file (without being pulled from a component databank) it is automatically assumed to have the properties of some material used as part of the New Component Definition Dialog. Such values may not be appropriate at all, resulting in significant errors in the simulation and/or economic viability of your process.

The fundamental component properties are clustered into seven groups:

- Pure Component: IDs
- Pure Component: Constant Physical Properties
- Pure Component: Temperature-Dependent Physical Properties
- Pure Component: Aqueous Properties
- Pure Component: Economic Properties
- Pure Component: Pollutant Categories.
- Pure Component: Comments

The aqueous group of component properties is related to the calculation of the environmental properties of streams; they are required by unit operation models typically needed in waste treatment and pollution reduction processes.

The pollutant categorization group of properties is related to the classification of a component as one of several classes of pollutants monitored by the US-EPA.

For processes where none of these issues is relevant, you can choose to ignore them without risking any impact on your simulation results.

PURE COMPONENT: IDS

Name	The formal name of a pure component. It is supplied when the component is originally introduced (either to the databank or the process file) and it cannot be edited later. It can be a string of up to 31 characters.
Local Name	The local name of a component is the display name (or ID) by which this component appears everywhere in the process (streams dialogs, operation dialogs, reports, etc.). It can be a string of up to 15 characters. It is supplied when the component is originally introduced (either to the databank or the process file), but it can be changed later (but must be unique). The name change cannot be done from the Pure Component Properties Dialog but from a a separate interface (select **Tasks ▸ Pure Components ▸ Rename** from the main menu to display the Rename Pure Component Dialog.
Trade Name	It keeps the name by which this component is widely known in the market. It is supplied when the component is originally introduced (either to the databank or the process file), but it can be changed later (but must be unique). It can be a string of up to 31 characters.
Formula	Represents the chemical formula of a pure component. It is provided when the component is originally introduced (either to the databank or the process file), but it can be changed later. Uniqueness is not required. It can be a string of up to 31 characters. The application does not parse the string to infer the component's molecular weight or any other properties. This string is merely kept for reference purposes only.
Chemical Abstract Serial Number (CAS Number)	The CAS of the pure component (if available). It is supplied when the component is originally introduced (either to the databank or the process file), but it can be changed later (but must be unique). It can be a string of up to 15 characters. For components whose CAS number is not available or doesn't exist (e.g. for all 'pseudo-components' like debris, biomass, etc.) the assigned number (string) is (by convention) always beginning with the characters "N/A" and then followed by a number.
Company ID	Often components are identified and tracked within corporations with a company-wide tag ID number. This field is reserved to contain exactly that description. It is provided when the component is originally introduced (either to the databank or the process file), but it can be changed later (uniqueness is not required). It can be a string of up to 31 characters.
Is Biomass?	The local name of a component is the display name (or ID) by which this component appears everywhere in the process (streams dialogs, operation dialogs, reports, etc.). It can be a string of up to 15 characters. It is supplied when the component is originally introduced (either to the databank or the process file), but it can be changed later (but must be unique). The name change cannot be done from the Pure Component Properties Dialog but from a a separate interface (select **Tasks ▸ Pure Components ▸ Rename** from the main menu to display the Rename Pure Component Dialog).

PURE COMPONENT: CONSTANT PHYSICAL PROPERTIES

Molecular Weight	Used in distillation, flash drum, condenser, absorber, and stripper, electrostatic precipitator, and all reactors. The molecular weight (MW) is used to convert amounts of that component from mass-unit to mole-units (as displayed on stream dialogs).
Enthalpy of Formation [J/gmol]	Used in steam generation. The (standard) enthalpy of formation specified at 25 ^{o}C is used as reference to determine the enthalpy of formation at the fuel temperature of a combustible fuel component or combustion product component.
Normal Boiling Point [^{o}C]	Used in distillation, flash drum, and condenser. It is commonly used as the default criterion for deciding the physical state of a component (Vapor or Liquid/Solid, see 8.12 Physical State Calculation Options).
Normal Freezing Point [^{o}C]	Not used in the current version of the program.
Critical Temperature [^{o}C]	Used by some rigorous VLE models (in distillation, flash evaporation, condensation, etc.)
Critical Pressure [bar]	Used by some rigorous VLE models (in distillation, flash evaporation, condensation, etc.)
Compressibility Factor	Used by some rigorous VLE models (in distillation, flash evaporation, condensation, etc.).
Acentric Factor (Omega)	Used by some rigorous VLE models (in distillation, flash evaporation, condensation, etc.)
Henry's Constant [atm-m3/mol]	Used in absorption/stripping and VOC emission calculations.
Particle Size [microns]	Used in filters and centrifuges
Default Volumetric Coefficient	Used in estimating the density of streams or vessel contents when the density model chosen is the volumetric contribution model (see 4.7d Stream Physical State Calculation Options).

PURE COMPONENT: TEMPERATURE-DEPENDENT PHYSICAL PROPERTIES

Density [kg/m3]	Used in converting between mass and volumetric flowrates and calculating the concentration of species in streams. For details, see ‘Density Calculation Options’ on page 8-25.
Liquid/Solid Heat Capacity [J/gmol-K]	Used in energy balances.
Gaseous Heat Capacity [J/gmol-K]	Used in energy balances.
Vapor Pressure [mm Hg]	Used in flash evaporation and condensation. It could also be used as a criterion for deciding the physical state of a component (Vapor or Liquid/Solid, see 8.12 Physical State Calculation Options).

Heat of Vaporization [J/gmol]	It estimates the heat of vaporization at any pressure (or temperature) estimated using Chen's method. It is used in energy balances when phase change is involved (e.g. flash evaporation and condensation). The user can either provide the values of Chen's correlation parameters (a & b) or ask them to be calculated based on the normal (at 1 bar) heat of vaporization using Watson's relation. (see 'The Properties of Gases and Liquids' by R.C. Reid, J.M. Prausnitz and B.E. Poling for details). The fundamental properties needed in these empirical formulas are the normal boiling point and the critical temperature and pressure.

PURE COMPONENT: AQUEOUS PROPERTIES

	Diffusiveness
Diffusivity in Water [cm2/s]	Used in VOC emission calculations.
Diffusivity in Air [cm2/s]	Used in VOC emission calculations.
	Bio-Degradation Properties
Kmax [mg substrate / g-biomass-h]	Maximum biodegradation rate constant. Used in biodegradation reaction rate calculations in the Aerobic BioOxidation.
Ks [mg/L]	Half-saturation constant. Used in biodegradation reaction rate calculations in the Aerobic BioOxidation.
	Oxygen Ratios
Chemical Oxygen Demand (COD) [g oxygen / g substance]	It represents the amount of oxygen (in g) required to chemically oxidize 1 g of the substance. It is used in calculating the COD value of material streams.
Theoretical Oxygen Demand (ThOD) [g oxygen / g substance]	It represents the theoretical amount of oxygen (in g) required for complete oxidation of 1g of the substance.
BODu/COD	It represents the ratio of the ultimate biochemical oxygen demand (BODu) to the COD of a substance. It is used in calculating the BODu value of material streams based on the COD value of each component.
BOD5/BODu	It represents the ratio of the five-day BOD to ultimate BOD. It is used in calculating the BOD5 value of material streams based on the BODu values.
	Nitrogen Ratios
Total Kjeldahl Nitrogen (TKN) [g TKN / g substance]	It represents the contribution of a component to total Kjeldahl nitrogen. It is used in calculating the TKN value of material streams.

Ammonia Nitrogen (NH3) [g NH3 - N / g substance]	It represents the contribution of a component to ammonia nitrogen. It is used in calculating the NH3 value of material streams.
Nitrate/Nitrite Nitrogen (NO3/NO2) [g NO3/NO2 - N / g substance]	It represents the contribution of a component to nitrate/nitrite nitrogen. It is used in calculating the NO3/NO2 value of material streams.
	Solids Ratios
IsSolid? [Boolean]	If TRUE, it indicates that this component is dissolved or suspended solid.
Total Solids (TS) [g solids / g substance]	It represents the fraction of a component that is dissolved or suspended solid (it will usually be either 0 or 1). It is used in calculating the TS value of material streams.
Total Suspended Solids (TSS / TS) [g TSS / g TS]	It represents the fraction of a solid component that is in suspension. It is used in calculating the TSS value of material streams. Naturally, 1.0 - TSS represents the dissolved fraction of the component.
Volatile Suspended Solids (VSS / TSS) [g VSS / g TSS]	It represents the fraction of the suspended amount of a solid component that is volatile. It is measured as the organic fraction that oxidizes at 550^{o}C and is driven off as gas. It is used in calculating the VSS value of material streams.
Degradable Volatile Suspended Solids (DVSS / VSS) [g DVSS / g VSS]	It represents the fraction of the volatile suspended solid amount of a component that is biodegradable. It is used in calculating the DVSS value of material streams.
Volatile Dissolved Solids (VDS / TDS) [g VDS / g TDS]	It represents the fraction of the dissolved solid amount of a component that is volatile. It is used in calculating the VDS value of material streams.
Degradable Volatile Dissolved Solids (DVDS / VDS) [g DVDS / g VDS]	It represents the fraction of the volatile dissolved solid amount of a component that is biodegradable. It is used in calculating the DVDS value of material streams.
	Other
Log10 (Octanol/Water)	The logarithm of the ratio of the concentrations of a component in octanol and water respectively. It indicates the hydrophobicity of a component and its tendency to associate with sludge. It is not used currently.
Total Organic Carbon (TOC) [g organic carbon / g substance]	It represents the contribution of a component to organic carbon. It is used in calculating the TOC value of streams.
Total Phosphorous (TP) [g phosphorous / g substance]	It represents the contribution of a component to total phosphorous. It is used in calculating the TP value of streams.

CaCO3 Ratio [g CaCO3 / g substance]	It represents the contribution of a component to total CaCO3. It is used in calculating the CaCO3 value of streams.

PURE COMPONENT: ECONOMIC PROPERTIES

Selling Price	Used in economic calculations.
Purchasing Price	Used in economic calculations.
Waste Treatment / Disposal Cost	Used to estimate the waste treatment/disposal cost of a waste stream based on its composition; if you do not provide a direct cost for waste treatment/disposal of the entire stream on a per-kg-mixture-basis, a cost is estimated based on the contribution to the cost of each component present.
Supplier	Records the name of the supplier (vendor) used to provide the material.

PURE COMPONENT: POLLUTANT CATEGORIES

Is Hazardous?	If TRUE, tags that component as hazardous. The presence of a hazardous component at a level higher than the hazardous threshold (see below) automatically tags the whole stream as hazardous.
Hazardous Threshold [PPM]	The concentration level above which the component renders a whole stream as hazardous.
SARA 313?	If TRUE, the component will be included in a SARA-313 chemicals section of the environmental impact report (EIR).
33/50?	If TRUE, the component is assumed to be in the 33/50 EPA program and as such it will be included in the 33/50 chemicals section of the environmental impact report (EIR).
Is Reported in Solid Waste Streams?	If TRUE, indicates that the component must be tracked in all solid waste streams and as such it will be present in the solid waste section of the EIR report.
Is Reported in Aqueous Waste Streams?	If TRUE, indicates that the component must be tracked in all aqueous waste streams and as such it will be present in the aqueous waste section of the EIR report.
Is Reported in Organic Waste Streams?	If TRUE, indicates that the component must be tracked in all organic waste streams and as such it will be present in the organic waste section of the EIR report.
Is Reported in Emissions?	If TRUE, indicates that the component must be tracked in all emissions and as such it will be present in the emissions section of the EIR and EMS reports.

If ‘Is Reported in Emissions?’ is TRUE, then the following more detailed pollutant categories may be specified:

- **Component Pollutant Primary Category**: One of: None (unregulated), VOC, Particulate, Acid Gas, ETG, CO, NOx, SO2, Base, or any of the user-defined categories.
  If a component is designated anything other than 'None', it will be included in the tallying up of the corresponding primary pollutant category as shown in the emissions section of the EIR report as well as the Emissions report. Note that if the user has defined his/her own categories of pollutants (through the Emission Limits Dialog) then these categories will appear as well under the 'Other' group of categories.
- **Components designated as VOCs**
  If a component is designated as a VOC then it must be further categorized. If it cannot be identified as belonging to any of the supplied 4 sub-categories (VCM, TVOS, EVOS or HAP-VOC), then it must be simply checked as 'other' VOC.
- **Components designated as Particulates**
  If a component is designated as a particulate then it must be further categorized. If it cannot be identified as belonging to any of the supplied 8 sub-categories (Biological, Radionucleid, Asbestos, Dioxin, LOC, HAP, Cr+6, Metal) then it must be simply checked as 'Other'. Limits for all above subcategories are specified by the EPA.
- **Components designated as Acid Gases**
  If a component is designated as an Acid Gas, then it must be further categorized as either HAP-Acid gas or non-HAP Acid Gas.
- **Component designated as ETGs**
  If a component is designated as an ETG, then it must be further categorized as either HAP-ETG or non-HAP ETG.

The aqueous group of component properties can only play a role in processes that focus on environmental impact (waster water treatment, air pollution control, etc.) they may be hidden if a user chooses to do so. This can be accomplished by visiting the document's context menu and selecting **Preferences ▸ Miscellaneous**...
Un -checking the related option will not only hide the "Aqueous Property' tab from the pure component.editing dialog, but will also hide the 'Env. Props' tab of all streams.

PURE COMPONENT: COMMENTS

Holds any documentation that may need to be conveyed to any engineers that may use this chemical. It may convey sources for the property values, precautionary measure that need to be taken when handling this chemical, etc.

There are detailed guidelines aimed at helping users to classify a material under one (or more) of the primary or secondary pollutant categories mentioned above (see Pollutant Categorization Guidelines). For each pollutant category, you can use the Emission Limits Dialog to specify allowable limits and SuperPro Designer will tally up the contributions from all emission streams of your process and will notify you of any violations.

For more on how to edit the properties of a registered component, see 'To edit the properties of a registered pure component...' on page 3-9. To find out how to edit the properties of a component in the databank, see 15.4a Viewing the Contents of the Pure Components Databank.

3.1f DIPPR Component Properties

In SuperPro Designer, you may use as a source of your component properties the DIPPR pure component databank. The DIPPR pure component database is developed and maintained by the Brigham Young University, and in its relational database contains a compilation from the open literature the physical and thermodynamic properties of over 1600 pure components.

Each property prediction, according to DIPPR, can be made using one of possible 8 different equations (correlations) as shown in Figure 3.2. The type of relation used as well as its constants can be modified (overwritten) by the user, if needed. SuperPro Designer provides access to a limited version of the DIPPR database (in relational database format). This is simply to demonstrate the ability of the program to access the DIPPR formatted component data as a third component databank. If you own the full DIPPR database, please visit the Databases: Availability, Password & Locations Dialog to make it available to SuperPro Designer.

For information on the DIPPR component property estimation models, see DIPPR Pure Component Properties Dialog: Physical (T-dependent) tab

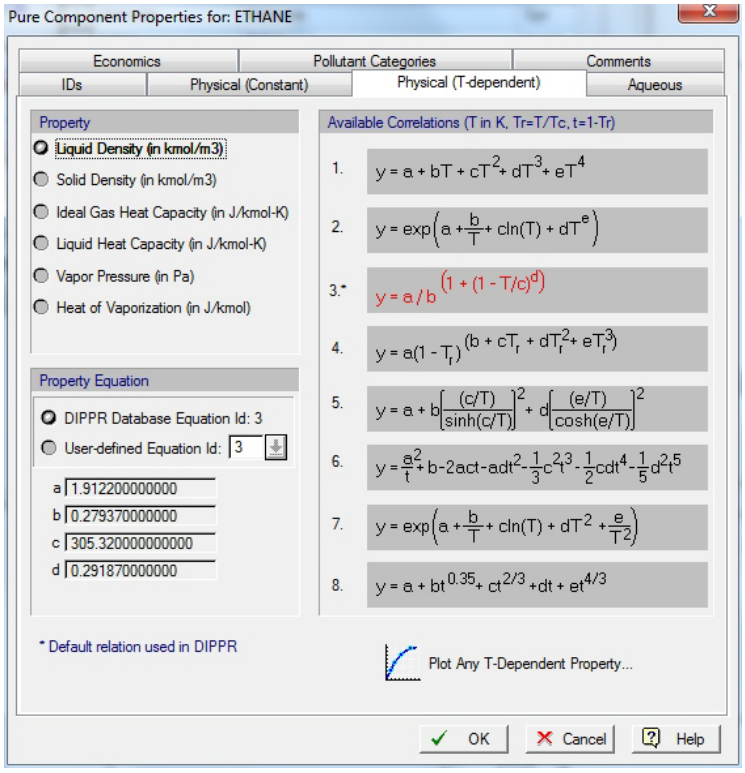
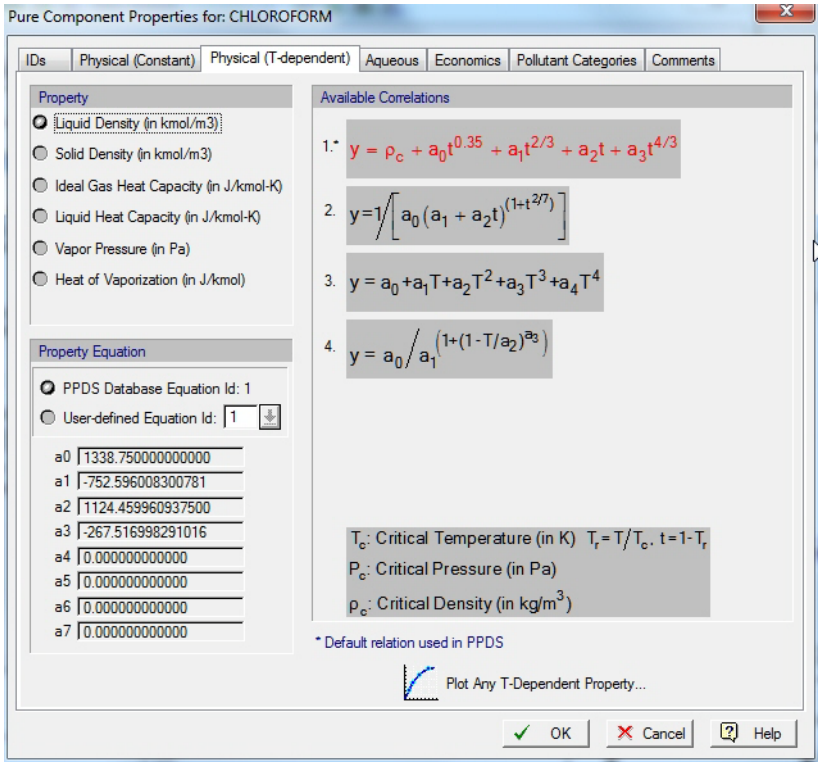

Pure Component Properties for: ETHANE
Economics
Pollutant Categories
Comments
IDs
Physical (Constant)
Physical (T-dependent)
Aqueous
Property
Liquid Density (in kmol/m3)
Solid Density (in kmol/m3)
Ideal Gas Heat Capacity (in J/kmol-K)
Liquid Heat Capacity (in J/kmol-K)
Vapor Pressure (in Pa)
Heat of Vaporization (in J/kmol)
Property Equation
DIPPR Database Equation Id: 3
User-defined Equation Id: 3
a 1.912200000000
b 0.279370000000
c 305.320000000000
d 0.291870000000
Available Correlations (T in K, Tr=T/Tc, t=1-Tr)
1. y = a + bT + cT^2 + dT^3 + eT^4
2. y = exp(a + b/T + cln(T) + dT^e)
3.* y = a / b^(1 + (1 - T/c)^d)
4. y = a(1 - Tr)^(b + cTr + dTr^2 + eTr^3)
5. y = a + b[(c/T)/sinh(c/T)]^2 + d[(e/T)/cosh(e/T)]^2
6. y = a^2/t + b - 2act - adt^2 - 1/3 c^2 t^3 - 1/2 cdt^4 - 1/5 d^2 t^5
7. y = exp(a + b/T + cln(T) + dT^2 + e/T^2)
8. y = a + bt^0.35 + ct^2/3 + dt + et^4/3
* Default relation used in DIPPR
Plot Any T-Dependent Property...
OK
Cancel
Help

Figure 3.2: Temperature dependent physical properties for DIPPR component.

3.1g PPDS Component Properties

There is a third choice for component properties. For users who own a copy of the PPDS pure component database, SuperPro Designer now allows them to introduce a component in a simulation with property values drawn directly from the PPDS component database. The PPDS component database is developed and maintained by a Scottish company (TÜV SÜD NEL) and

it must be purchased separately. For users who own a copy of PPDS, they can introduce it to SuperPro Designer by visiting the Databanks Availability, Passwords and Location Dialog (**Databanks ▸ Availability, Passwords and Location...**.) For such components, the T-Dependent property tab appears as follows:



As it can be seen, PPDS supports a different set of empirical correlations. Users can accept (for a given property as selected at the top right) the correlation as provided by the database, or they can switch to another relationship and provide their own parameters.

3.1h Synchronize Registered Component Properties with Databank

It often becomes necessary to realign the component properties of materials as they exist in your process file with their records in the databanks where they originally resided. There may be several reasons for that. You may have experimented with different values for some of their properties but in the end, you realize that you were better off keeping the original values. Or, as you were developing your process simulation, some other members of your organization may have updated the database records for some of the components engaged in your simulation. Sometimes, you may want to move the date in the other direction: from your components as they now exist in your process file, back into their permanent records in the databank. Perhaps you experimented with slightly different values for some of their properties and as it turns out, they describe their behavior more accurately. Or, perhaps you imported their values from a someone else's 'User' database file that is no longer accessible to you but you wish to keep a permanent record in your own databank.

This synchronization between your own component objects and the databank records can be done by using two dedicated interfaces for this purpose:

(a) To update your component properties from the databank records, select **Tasks ▸ Pure Components ▸ Update Properties From DB** from the main menu of the application and work with the Update Pure Component Properties From the Databank interface.

(b) To update the databank records based on the values of the component objects as they are currently in your process file, select **Tasks ▸ Pure Components ▸ Update Properties to DB** from the main menu of the application and work with the Update Pure Component Properties To the Databank interface.

3.1i Component Properties in a Binary Mixture

By default, SuperPro Designer uses Raoult's law as the default option for calculating the physical state of material with the rigorous Toolbox. Such calculations require pure component data only. Specifically, they require the estimation of a pure component's vapor pressure at a given temperature (Antoine's coefficients typically are used that estimation). In situations where components and conditions are such that Raoult's law no longer produces satisfactory results, users have the option to employ more sophisticated VLE models, see Appendix D (Vapor-Liquid Equilibrium Modeling). These VLE models attempt to capture the non-ideal behavior of the vapor and liquid phase with increased accuracy by employing binary interaction coefficients. These coefficients participate in the following equations of state (see D.2 Equations Of State (EOS) for details):

- Virial
- Peng Robinson
- Soave-Redlich-Kwong

and the following activity coefficients models (see D.3 Activity Coefficient Models):

- Wilson
- NRTL (g_{ij}, g_{ji})
- NRTL (a_{ij})

The 'Designer' databank includes binary interaction coefficients for over 60 binary mixtures and users can add their own data in the 'User' portion of the databank. For more information on binary coefficient databanks, see 15.6 Binary Coefficients Databank.

BINARY CHARTS

When engaging non-ideal models to predict the vapor-liquid split of several components, it is critical to make sure that the model chosen produces sufficiently accurate values for each binary component combination on its own. If the binary behavior is not captured accurately, then there's little hope that the predictions for the entire mixture will be accurate. SuperPro Designer allows you to view binary x-y diagrams generated based on your choice of model (see Vapor-Liquid Equilibrium Modeling) and the values of b_{ij} (binary coefficients) provided through the .

For information on the interface used to choose VLE options such as fugacity models, and specify the binary coefficients for each method, see The Rigorous PS Calculation Toolbox Dialog.

3.2 STOCK MIXTURES

A stock mixture is simply a mixture of pure components and/or other stock mixtures with a given composition (in mass or molar percentage). Typically stock mixtures are used to represent materials that are provided and consumed by a process 'as-is' in the form of a mixture. Examples of such process consumables might be buffers, acid solutions, base solutions, etc. Stock mixtures can be used to initialize process input streams (see 4.7b Composition & Related Properties of a Bulk Input Stream) or they can be employed directly by an operation (without being present on any stream) as special agents (e.g. in a 'Clean-in-Place' (CIP) operation as a cleaning agent, in a 'Gas Sweep' operation as a sweeping agent, etc.) The most important property descriptions that you need to provide for a mixture is its composition and its price (see 3.2d Stock Mixture Properties). In order to facilitate the reuse of mixtures without having to describe all their properties from scratch each time, the application keeps a list in a stock mixture databank (see 15.5 Databank of Stock Mixtures). Before a stock mixture can be engaged by your process simulation, it needs to be introduced (registered, see 3.2a Stock Mixture Registration) and be given a name-ID ('Local Name') that will be used to represent the mixture.

Since stock mixtures can only be used as inputs to a process, they only exist to describe the composition of input streams of a process. You will never find the names of mixtures as part of the composition description of an intermediate or output stream. Stock mixtures lose their identity once they are come in contact with other mixtures or pure components. SuperPro Designer converts mixture flows into their equivalent pure component flows and performs material balances and reports results based on pure component flows and compositions.

3.2a Stock Mixture Registration

In order to make a stock mixture available to be used as an ingredient in the composition of an input stream in your process, you must first register it. Registering a stock mixture, (just as registering a component) simply means that you introduce this mixture into your process file and provide an accurate description of its properties. You may register a mixture simply by importing it (and thereby copying all its properties) from the stock mixture databank (in the 'Designer' or the 'User' database). Alternatively, you may introduce an altogether new mixture that does not exist (currently) in the stock mixture databank. These options are exactly analogous to options available for pure components (see 3.1a Pure Component Registration).

Mixtures can be registered through the dialog that appears when you select **Tasks ▸ Stock Mixtures ▸ Register, Edit/View Properties** form the main menu of the application (or type **Ctrl+Shift+0** as a shortcut). This selection will bring up the Stock Mixture Registration Dialog. Registering a new stock mixture serves mainly two purposes:

1. Provide to the process simulation a description of all of the mixture's properties (composition, density, price, etc.), and

2. Define a short name tag (‘Local Name’) which will be used everywhere the application needs to reference the mixture (on stream initialization dialogs, reports, etc.). Please note that each registered mixture’s ‘Local Name’ must be unique among all registered stock mixtures and pure components.

After a stock mixture is registered, you can still edit its properties (see ‘To edit the properties of a registered mixture...’ on page 3-25). Note that the ‘Name’ cannot be edited; the ‘Local Name’ can be edited but not from the Stock Mixture Properties Dialog. You need to visit the Rename Stock Mixture Dialog to change the ‘Local Name’ of a stock mixture after it has been registered.

3.2b Stock Mixture Registration Dialog

This dialog appears when you select **Tasks ▸ Stock Mixtures ▸ Register, Edit/View Properties** from the main menu of the application

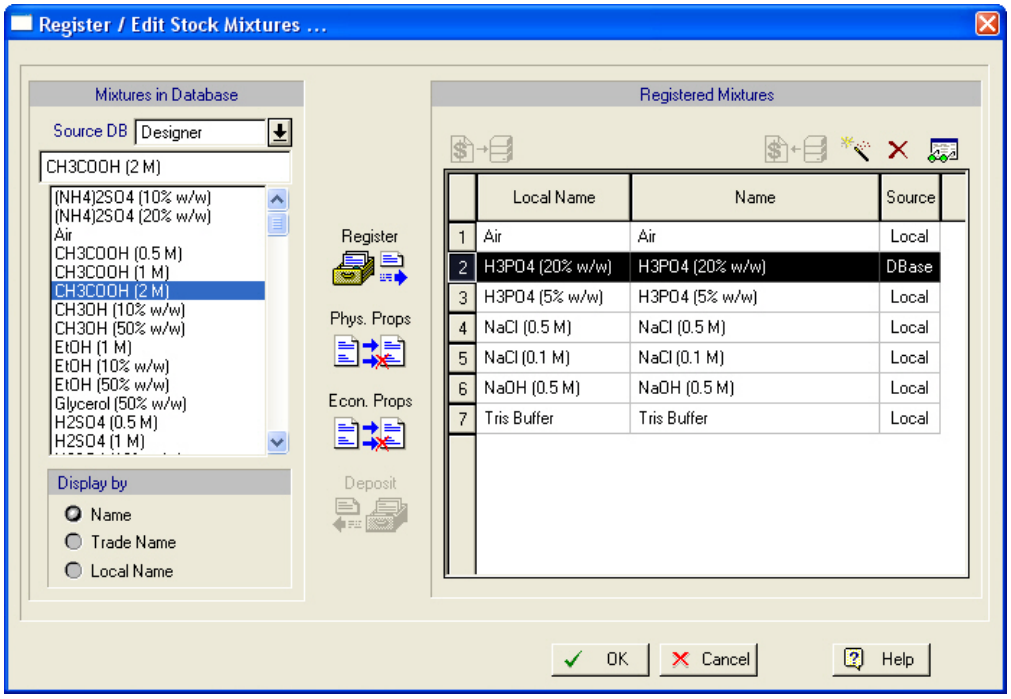


Figure 3.3: The stock mixture registration dialog.

Using the interface shown in Figure 3.3 you can:

- Introduce (register) a new stock mixture into the process by importing it from a stock mixture databank.
- Introduce (register) an altogether new stock mixture (which does not exist in any of the stock mixture databanks.)
- Delete an already registered stock mixture.
- Edit the properties of a registered stock mixture.

- Deposit a stock mixture already registered in your process to the stock mixture databank so that it can be used later by you or any other member of your team.
- Transfer (copy) the physical or economic property data (kept in the 'Designer' or 'User' portion of the stock mixture databank) from a member of that databank onto an already registered mixture that either lacks such data or has outdated data.
- Reconcile (synchronize) the property values of a registered mixture with its values in the databank (requires that the mixture still has a databank record).

Every registered mixture is identified within your process by a 'Local Name'; that is simply a short name by which this mixture will be mentioned in any input stream initialization dialogs or any stream reports related to this process simulation.

▶ To register a stock mixture by importing it from the mixture databank...

1. Select the source database.
   From the top left list box select the source database ('Designer' or 'User'). Notice that after you make a selection, the listbox below is populated with the names of mixtures in the selected database.
2. Select the mixture from the displayed listing.
   From the databank contents list box, select the mixture that you want to pull into the process. If the name is not visible, you may scroll up or down until you locate it, or start typing the name at the top of the list box. Notice that as you start typing the name of the mixture you wish to locate, the program responds by automatically scrolling in order to find and select the first choices that matches the typed portion of the name. The mixture databank contents may be listed by any of the following indices: 'Name', 'Trade Name' or 'Local Name'.
3. Click on the **Register** button.

   Notice that the number of rows in the registration table will expand by one. The mixture order may change as mixtures are listed alphabetically based on their 'Local Name'.
4. If you wish to view and/or edit any of the mixture properties see 'To edit the properties of a registered mixture...' on page 3-25.
5. Repeat steps 1 through 3 for all mixtures that you wish to register, then exit the Stock Mixture Registration Dialog by clicking on the **OK** button.

If the mixture you are about to register requires the presence of ingredients that are not still registered, SuperPro Designer will automatically register (after the user's approval) all such pure components and/or other stock mixtures. You cannot have a stock mixture present in a process simulation without all of its ingredients being present (registered) as well. Also, if you attempt to delete from the registration list any such ingredient (while still being used in the description of a registered stock mixture), the application will not allow it.

▶ To register a new stock mixture (not residing in a mixture databank) in your process simulation...

1. Click on the **Create New** ( ) button.
   Fill in the fields of the New Stock Mixture Definition Dialog that comes up. Even though uniqueness of names is strictly required amongst all other mixtures in your file, it is recommended that you supply names that are unique amongst the whole 'User' database, in case you later decide to keep the mixture and deposit it there.
2. Specify how property values will be initialized.
   Before the new mixture is introduced to your process, the application needs to know how to initialize its properties. You have two choices:
   (a) select another mixture to be used as source, or
   (b) request that all mixture properties are set to zero.
   Choice (b) will force you to visit the mixture's properties dialog in order to provide proper values (see 'To edit the properties of a registered mixture...' on page 3-25) before you exit the registration dialog.
3. Click **OK**.
   Unless the program detects any conflicts with the 'Local Name' specification, the new mixture will be added to the list of registered components. If you choose to keep the new mixture definition and have it available for use by a future project, you should deposit this mixture in your mixture databank (see 'To deposit a registered stock mixture into the mixture databank...' on page 3-26).

▶ To edit the properties of a registered mixture...

1. Select the mixture in the registration table
   Locate the mixture in the registration table, and click on the row that represent the mixture. Notice that when you click on it, the whole row is highlighted.
2. Click on the **View/Edit Properties** ( ) button
   The Stock Mixture Properties Dialog will appear. From that dialog you can edit the mixture's properties. For a complete description of the mixture properties, see 3.2d Stock Mixture Properties.
3. To keep the changes you made on the selected mixture's properties, exit the Stock Mixture Properties Dialog by clicking on **OK**. The changes are still not permanent. They will become permanent when you exit the Stock Mixture Registration Dialog by clicking **OK**. If you don't exit the Stock Mixture Registration Dialog with **OK** but by clicking **Cancel**, any mixture property modifications you made will be lost.

Modifying the properties of a registered stock mixture that was pulled from a mixture databank does not affect the property values of the original mixture record in the databank. It also will not affect the mixture properties of the same mixture used in simulations by others sharing the same mixture databank(s) with you.

▶ To delete a registered stock mixturet...

1. Select the mixture in the registration table
   Locate the mixture in the registration table and click on the row that represents the mixture. Notice that when you click on it, the whole row is highlighted.
2. Click on the **Delete** the ✕ button.

▶ To deposit a registered stock mixture into the mixture databank...

1. Select the mixture in the registration table
   Locate the mixture in the registration table, and click on the row that represent the mixture. Notice that when you click on it, the whole row is highlighted.
2. Make sure that 'User' is displayed at the top-left list box as the 'Source Database'.
3. Click on the **Deposit** button

   If the component does not exist in the 'User' database currently, it will be added. If the component already exists in the database, the program will request a further confirmation that indeed the intention is to update the existing component properties in the databank. In any future project that you may need to import that component from the databank, the component will have the newly assigned set of values.

*Please remember that any changes in the 'User' database as a result of any action on this dialog will be permanent and will not be reverted even if you exit the dialog with **Cancel**.*

▶ To copy only subset of mixture properties...

1. Select the target stock mixture in the registration table.
   Locate the mixture in the registration table, and click on the row that represent the mixture. Notice that when you click on it, the whole row is highlighted.
2. Select a 'Source Database'.
   Select one of the databases ('Designer' or 'User') and notice how the table below fills up with the contents of its mixture databank.
3. Select the source stock mixture.
   From the contents of the selected database, select the mixture you wish to use as the source of the mixture properties.
4. Click on **Phys Props** or **Econ Props** button.
   If you wish to copy the physical properties of a mixture, then click on the **Phys Props** button. If you wish to copy the economic properties then click on the **Econ Props** buttons.

▶ **To synchronize the economic properties of a registered mixture with its databank record...**

1. Select a registered mixture which exists in the 'User' database. In order for a mixture to be verified as 'existing' in the 'User' database, its 'Name' must match exactly with one of the records in that databank.
2. Click on the **Update Econ. Data from DB** ( ) button to update the economic properties of the registered stock mixture from the record in the 'User' database.
3. Click on the **Update Econ. Data in DB** ( ) button to update the economic properties of the mixture record in the 'User' databank based on the current values of the registered mixture. Please remember that any changes in the 'User' database as a result of this action will be permanent and will not be reverted even if you exit the registration dialog with **Cancel**.

3.2c Pre-Registered Mixtures

As soon as you start a new process simulation project, SuperPro Designer introduces (registers) automatically for you one stock mixture: 'Air'. The reason that 'Air' is automatically introduced is because typically, all vessels are assumed to be filled with air at the start of a simulation run (before any liquid contents are transferred in). In order for 'Air' to be registered, SuperPro Designer also auto-registers the pure components that are the ingredients for 'Air': 'Oxygen' and 'Nitrogen' (see Pre-Registered Components). Note that 'Air' cannot be deleted from the list of registered mixtures.

3.2d Stock Mixture Properties

Stock mixtures have very few properties as they only have a temporary presence at entry points of the process. Their properties are presented for viewing and/or editing on the Stock Mixture Properties Dialog in four groups:

- Stock Mixture: IDs
- Stock Mixture: Composition & Density
- Stock Mixture: Economics
- Stock Mixture: Comments

STOCK MIXTURE: IDS

Name	The formal name of a stock mixture. It is supplied when the mixture is originally introduced (either to the databank or the process file), and it cannot be edited later. It can be a string of up to 31 characters. Should be unique amongst all other mixtures and components in the databanks.

Local Name

The local name of a mixture is the display name (or ID) by which this mixture appears everywhere in the process (streams dialogs, operation dialogs, reports, etc.). It can be a string of up to 15 characters. It is supplied when the mixture is originally introduced (either to the databank or the process file), but it can be changed later (but must be unique). The name change cannot be done from the Stock Mixture Registration Dialog but from a a separate interface (select **Tasks ▸ Stock Mixtures ▸ Rename** from the main menu to display the Rename Stock Mixture Dialog.

Trade Name

It is meant to display a name by which this mixture is widely known in the open market. It is supplied when the mixture is originally introduced (either to the databank or the process file), but it can be changed later (but must be unique). It can be a string of up to 31 characters.

STOCK MIXTURE: COMPOSITION & DENSITY

Composition

The composition of a mixture described on a mass or molar basis. A mixture can be composed of pure components as well as of other mixtures. All of the mixture's ingredients must be present in the same environment as the mixture: if the mixture is a registered mixture, then all of its ingredient must be registered in the same process file; if the mixture is present in a databank, then all of its ingredients must be present in either the 'Designer' or 'User'portion of the component databank.

If the composition of the mixture is not known but the concentration of one (or more) key ingredients is (as molarity or strength in one or more components) you may find it useful to use the target concentration calculator feature available on the Stock Mixture Properties Dialog: Composition Tab.

Density

The density of a mixture is calculated based on a user-selected model. There are three models that users can choose from:
a) A parametric model: D (in g / L) = a + bT (T in K)
b) Assuming that the mixture will always be used in liquid/solid state, use a composition-based weighted average of the liquid/solid density estimates of its ingredients, or

c) Ideal gas law (assumes that the mixture is always in gaseous state).

The mixture's density is only used when the mixture is the one and only ingredient of an input stream and the stream's density model dictates to use its ingredients as source (see 4.7d Stream Physical State Calculation Options).

STOCK MIXTURE: ECONOMICS

Purchase Price $/base-unit	It can be either be provided directly by the user (on a per-unit-of-choice basis) or it can be calculated from the mixture's ingredients as the weighted average of their purchasing price. The basis units are 'kg' by default but may be changed by the user to any one of several choices of mass or volume units. If a a per-volume choice is made (e.g per-gallon), then to convert the price on a per-mass basis, the application will use its density model to compute the density of the material in 0 and 1 bar.
Supplier	Preserves the name of the most common supplier for this chemical. Kept for documentation purposes only.

STOCK MIXTURE: COMMENTS

Holds any documentation that may need to be conveyed to any engineers that may use this chemical. It may convey sources for the property values, precautionary measure that need to be taken when handling this chemical, etc.

To find out how you can edit the properties of a registered stock mixture in a process, see 'To edit the properties of a registered mixture...' on page 3-25. To find out how to edit the properties of a stock mixture in the databank, see 15.5a Viewing the Contents of the Stock Mixtures Databank.

3.2e Synchronize Registered Stock Mixture Properties with Databank

It often becomes necessary to realign the mixture properties of materials as they exist in your process file with their records in the databanks where they originally resided. There may be several reasons for that. You may have experimented with different values for some of their properties but in the end, you realize that you were better off keeping the original values. Or, as you were developing your process simulation, some other members of your organization may have updated the database records for some of the mixtures engaged in your simulation. Sometimes, you may want to move the date in the other direction: from your mixtures as they now exist in your process file, back into their permanent records in the databank. Perhaps you experimented with slightly different values for some of their properties and as it turns out, they describe their behavior more accurately. Or, perhaps you imported their values from someone else's 'User' database file that is no longer accessible to you but you wish to keep a permanent record in your own databank.

This synchronization between your stock mixture objects in a process file and the databank records can be done by using two dedicated interfaces for this purpose:

(a) To update your component properties from the databank records, select **Tasks ▸ Stock Mixtures ▸ Update Properties From DB** from the main menu of the application and work with the Update Stock Mixture Properties From the Databank interface.

(b) To update the databank records based on the values of the mixture objects as they are currently in your process file, select **Tasks ▸ Stock Mixtures ▸ Update Properties to DB** from the main menu of the application and work with the Update Stock Mixture Properties To the Databank interface.

4

STREAMS

Streams represent the flow of bulk material (as bulk streams, see 4.7 Bulk Streams) or discrete entities (as discrete streams, see 4.8 Discrete Streams) from one unit procedure to the next. Streams can be direct process inputs, intermediates or outputs (see 4.1 Types of Streams). All attributes of input streams (composition, temperature, pressure, etc.) must be initialized by the user (see also 4.9 Auto-Initialization of Input Streams) whereas the main attributes of intermediate and output streams are calculated by the application after the mass & energy (M&E) balances are executed. Streams are displayed on the process flowsheet as polylines made up strictly of horizontal and/or vertical segments. When drawing a stream, always start from the source and finish with the destination (see 4.10 Classification of Input and Output Streams). After each stream is drawn, it is assigned a name that is generated using a automatically by the application using a prefix (like "S-") and a number (see 8.20h Automatic Name Generation). The chosen name is displayed on a name tag (see 4.5 Stream Tags). The name tag is automatically positioned by the application (but can be adjusted by the user, if need be) and moves automatically when the stream's shape changes. The auto-generated name can be changed by the user after the stream is created. A string can be given any name so long as it is unique among all stream names in the process. The appearance of streams (line color, thickness, location of name tag, etc.) is all kept by a stream style object (see 4.6 Stream Style). The default stream style for bulk and discrete streams is kept by the process file and can be changed by the user (see 8.3 Default Style for Process Elements). Also, individual streams can have their style modified if so desired through the Stream Style Dialog.

4.1 TYPES OF STREAMS

Depending on the nature of the material that is represented by a stream, SuperPro Designer distinguishes between two types of streams:

(a) Bulk Streams

(b) Discrete Streams

Bulk streams carry material measured by flowrate units:
(mass-or-volume units) / (time units), or (mass-or-volume units) / batch.
Part of the material can be in liquid, gaseous or solid phase but SuperPro Designer distinguishes only two phases: liquid/solid and vapor. The flow of **discrete streams** on the other hand, is measured in:
(Entities) / (time units) or (Entities) / batch.
Each discrete stream carries one and only one type of entity (e.g. '12oz Plastic Bottle'). The definition of the entity carried by an input stream is done as part of the initialization of the

stream (see 4.8b Discrete Input Streams). For intermediate or output discrete streams, the definition and description of the entity carried by the stream is inferred (or retrieved) from the operation in the procedure that originally produces the entity. When streams are connected to a unit procedure (as their source or destination), they are attached to one of its input or output ports (see 5.5 Unit Procedure Ports). Bulk streams can only be attached to bulk-stream ports and discrete streams can only be attached to discrete-stream ports.

You do not have to explicitly set the stream type as bulk or discrete. SuperPro Designer automatically decides their type based on the context (type of port that it is connected). If you start a stream by clicking on a procedure's output port, SuperPro Designer automatically creates the correct stream type (bulk or discrete) depending on the type of the port that you started. When creating an input stream, SuperPro Designer will decide the nature of the stream only after you have clicked on a destination port. The application will not allow you to hook-up a discrete stream to a bulk port and vice versa.

Every stream must have either a source or a destination procedure or both. There can't be a stream that has no source and no destination procedure. Based on the presence or absence of a source and/or a destination procedure, a stream is characterized as:

(a) **Input Stream**: a stream that has no source procedure.

(b) **Intermediate Stream**: a stream that has both a source and a destination procedure.

(c) **Output Stream**: a stream that has no destination procedure.

For input streams, most of their properties (such as pressure, temperature, flow and composition) must be specified by the user. All properties of intermediate and output streams are calculated as part of the simulation results (after the M&E balances are executed) and they cannot be edited by the user. The only attributes of intermediate streams that can be edited are those related to the determination of the physical state of the stream and its density (a.k.a, **the Physical State Toolbox**). This is done through the Bulk Intermediate/Output Stream Dialog: Physical State Tab.

When viewing the composition of output or intermediate streams on their i/o dialog (see 4.7a Viewing and Editing the Simulation Data of Bulk Streams), components with zero flowrates are not reported. Input streams on the other hand will display all ingredients introduced in the composition table (regardless of their assigned flow value).

From the standpoint of process economics, streams contribute differently depending on how they are classified. SuperPro Designer considers the following nine types of classifications for streams:

(a) Raw Material

(b) Revenue or Credit

(c) Cleaning Agent

(d) Waste (Solid Waste, Organic Waste, Aqueous Waste, or Emission)

(e) None (Un-classified).

Only input streams can be classified as 'Raw Material' and only output streams can be classified as 'Waste' (of any type). Unlike the previous stream types (bulk vs discrete and input vs output/intermediate) that are automatically assumed by the application based on the inherent nature of the stream, the economic stream classification must be done explicitly by the user. For more details, see 4.10 Classification of Input and Output Streams.

4.2 STREAM DRAWING

If you plan on drawing several streams, one after another, it is easier if you switched to **Connect Mode**. To enter the connect mode, click on the connect button displayed on the main toolbar. Notice that the cursor changes into the 'Connect Mode Cursor', to remind you, that the system is now in connect mode:

: The Connect Mode Cursor.

Remember that when you draw a stream you always start from the source and then conclude the drawing at the destination of the stream. For input streams, without a source procedure, you start from an unoccupied area of the flowsheet. For output streams, without a destination procedure, you end at an unoccupied area of the flowsheet. After you start the process of drawing a stream, you can either add your own elbows to give a custom-appearance to all the stream segments, or you can directly end the stream by designating its destination point (and let the application auto-draw the stream segments.) For step-by-step instructions on how to draw an input, intermediate or output stream see below.

- To draw an input stream...
- To draw an intermediate stream...
- To draw an output stream...

The system remains in connect mode after a stream has been created in order to allow you to create the next stream. When you are finished drawing streams, you should return to **Select Mode** by clicking on the select button of the main toolbar. The select mode cursor will appear:

: The Select Mode Cursor

▶ To draw an input stream...

1. Make sure you are in connect mode (the button is pressed o the main toolbar).
2. Since you are always drawing streams source-to-destination but input streams do not have a source procedure, move the mouse to an unoccupied area of the flowsheet (where you wish to start the drawing of the input stream) and click *once* to start the drawing the first segment of the input stream. The first segment can either be horizontal or vertical.
3. Move the mouse to draw either a vertical or a horizontal segment for the stream. *Do not hold the mouse pressed down as you are moving it to create the segment*. Notice that you don't have to be exact in your horizontal or vertical motion with the mouse as the system always draws either horizontal or vertical segments (approximating the exact location of the mouse to the nearest horizontal or vertical location).
4. A *single mouse click* ends the current segment and starts another one. The next segment must alternate its orientation. In other words, if the previous segment was horizontal, then this segment must be vertical and vice versa.
5. Repeat steps (2) through (4) to give the desired shape of the stream by adding extra segments (if so desired).

6. End the stream by a *single click* on an unoccupied input port. Note that an input stream cannot end with a vertical segment.

▶ To draw an intermediate stream...

1. Make sure you are in connect mode (the button is pressed o the main toolbar).
2. Since you are always drawing streams source-to-destination, move the mouse over an unoccupied output port (cursor changes to double direction arrow) and click *once* to start the drawing of the first segment of the stream. The first segment of an intermediate stream must be a horizontal segment.
3. Move the mouse to draw either a vertical or a horizontal segment for the stream. *Do not hold the mouse pressed down as you are moving it to create the segment*. Notice that you don't have to be exact in your horizontal or vertical motion with the mouse as the system always draws either horizontal or vertical segments (approximating the exact location of the mouse to the nearest horizontal or vertical location).
4. A *single mouse click* ends the current segment and starts another one. The next segment must alternate its orientation. In other words, if the previous segment was horizontal, then this segment must be vertical and vice versa.
5. Repeat steps (2) through (4) to give the desired shape of the stream by adding extra segments (if so desired).
6. End the stream by a *single click* on an unoccupied input port of the destination procedure. Note that an intermediate stream cannot end with a vertical segment.

▶ To draw an output stream...

1. Make sure you are in connect mode (the button is pressed o the main toolbar).
2. Since you are always drawing streams source-to-destination, move the mouse over an unoccupied output port and click *once* to start drawing the stream. Notice that the first segment of the stream must be a horizontal segment.
3. Move the mouse to draw either a vertical or a horizontal segment for the stream. *Do not hold the mouse pressed down as you are moving it to create the segment*. Notice that you don't have to be exact in your horizontal or vertical motion with the mouse as the system always draws either horizontal or vertical segments (approximating the exact location of the mouse to the nearest horizontal or vertical location).
4. A *single mouse click* ends the current segment and starts another one. The next segment must alternate its orientation. In other words, if the previous segment was horizontal, then this segment must be vertical and vice versa.
5. Repeat steps (2) through (4) to give the desired shape of the stream by adding extra segments (if so desired).
6. Since a single click will introduce an elbow, and an output stream must end on a point that is not an input port, you must *double click on an empty area of the flowsheet to terminate the drawing of an output stream*. You can end an output stream on either a horizontal or a vertical segment.

When you are in the midst of drawing a stream and the stream segment being drawn reaches the end of the viewable area, SuperPro Designer will automatically scroll in the direction where the mouse is moving in order to allow you to view more of the flowsheet area without interrupting the stream drawing procedure.

While in select mode, if you want to draw just one stream and then immediately go back to select mode, you may find it easier instead of switching to connect mode, to switch to the **temporary connect mode**. While in select mode, you can enter the temporary connect mode by holding down the **Ctrl** key and double-clicking with the mouse over an output port (to start an intermediate or output stream) or over an empty area (to start an input stream). Unlike what happens when ending a stream while in connect mode, this time, immediately after the stream is created, the system will revert to select mode.

NOTES

(a) Every time a stream touches upon an icon's port, its segment must be horizontal. Therefore the first and last segment of an intermediate stream must be horizontal; the last segment of an input stream must be horizontal; the first segment of an output stream must be horizontal.

(b) Every icon's port can only host one stream. You cannot start a stream from an output port that already has a stream attached to it, and you cannot end a stream on an input port that has a stream attached to it.

(c) When starting to draw an stream from a bulk output port of procedure, the application assumes you are about to draw a bulk stream, and it will not allow you to end it on a discrete input port. Similarly, when you start drawing a stream from a discrete output port of a procedure, the system assumes that you are about to create an intermediate discrete stream, and it will not allow you to end it on a bulk input port.

(d) You do not have to draw every segment of a stream. If the location of stream elbows is not important, you can simply initiate the drawing of the stream and then skip straight to the step that ends the stream. The application will automatically create the minimum number of segments needed to bridge the two points and insert the stream. A word of caution is necessary: the auto-connect algorithm may introduce stream segments that could cross over other streams or run over procedure icons. It is not recommended that you use this shortcut when drawing streams in a crowded flowsheet.

(e) During drawing of any stream segment, while left click introduces a new elbow, a right click removes the last elbow of the stream. After a stream has been drawn, the location of its elbows can be edited (see 4.4 Stream Elbow Editing).

(f) During drawing of any stream, hitting **Esc** aborts the whole procedure.

▶ To delete a stream (or any other item on the flowsheet)...

1. Make sure you are in select mode (the button is pressed on the main toolbar).
2. Click on the item that is to be deleted in order to select it (notice how the items is now shown in red color). If you wish to delete multiple items, then either group-select them (by

click-and-dragging a selection rectangle around them) or keep adding items to the selection group one-by-one by clicking on them while holding the **Ctrl** key down. Note that if you **Ctrl**+click on an item already selected it will be removed from the group of selected items.

3. Click on the **Delete** button (✕) on the main toolbaor, or hit the **Delete** or **Backspace** key on your keyboard. If procedure icons are part of your deletion group, you may be warned if their deletion (including their contained operations) may affect the settings of other operations in the process. If you refuse to proceed with the deletion (by click No on the warning dialog that appears) then the deletion of the selected items will be cancelled. If there was no warning or you allowed the system to proceed with the deletion by clicking on Yes in the warning dialog, then all selected items will be deleted from the flowsheet.

When a unit procedure icon is deleted from the flowsheet, all streams attached to it will also automatically be deleted as well.

There is no Undo option in SuperPro Designer. Every modification (including deletion of items) applied to your process cannot be undone unless you revert to the last saved version of the process. If you have made some inadventent changes to your process and saved the file, you may still be able to revert to an older version (see 8.19c Automatic Versioning (Archiving) of the Process File). When tackling a large project, it is highly recommended to keep several versions of your project in distinct files ("ProjectX.v1.spf", "ProjectX.v2.spf", etc., see 8.19b Working on a Long Term Project).

4.3 THE STREAM'S CONTEXT (OR COMMAND) MENU

If you move your cursor over a stream it will turn into: : The Command Menu (or Context Menu) Cursor indicating that if you right-clicked over that stream, you will be presented with a menu of commands. This menu is called the **stream's command menu** (or context) menu; sometimes, it is simply called the stream's right-click menu (see Figure 4.1). The menu includes commands that can be issued to the stream under the mouse.

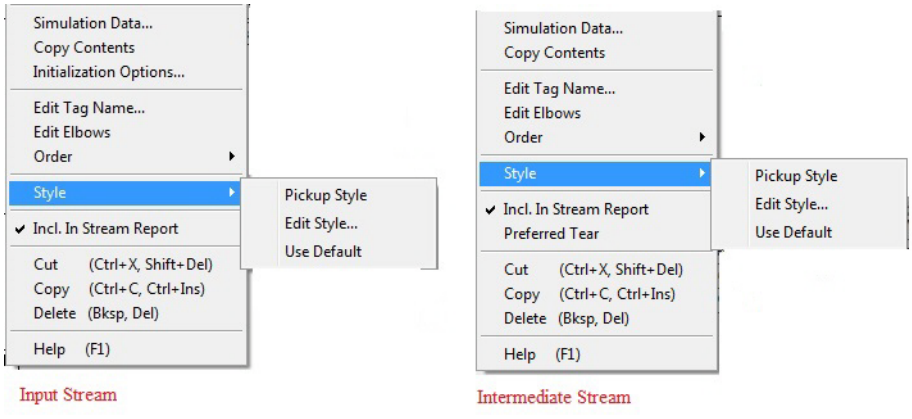


Figure 4.1: The command (context) menu for an input and an intermediate/output stream.

As you can see from the figure above, the contents of the menu may be slightly different depending on the type of stream (input, output or intermediate) and its particular connectivity

(e.g. if it is on a loop, see 8.14g Loop Identification and Tear Stream Selection). It is also possible to select multiple streams (select one, then **Shift+Click** to add to the selection list) and then present the command menu of one of the stream's in the selection list. In that case, the contents of the menu will include only those commands that can be applied to all streams currently selected.

4.4 STREAM ELBOW EDITING

After a stream has been introduced, you cannot click-and-drag it to move it on the flowsheet on its own. On the other hand, you can move unit procedure icons. After a unit procedure icon (with streams attached to it) has been moved, the application will automatically adjust the location of some of the attached streams' elbows in order to guarantee that its segments are always strictly horizontal or vertical. If the new location of the stream's elbows is not satisfactory, you can edit them.

▶ **To relocate the stream's elbows...**

1. Make sure you are in select mode (the button is pressed on the main toolbar).
2. Move the mouse over the stream whose elbows you wish to edit and select **Edit Elbows** from the stream's command menu. Notice the appearance of small black rectangles (called **elbow handles**) right over the current location of the stream's elbows.
3. Move the mouse over an elbow handle. Notice how the cursor changes shape into a double arrow that shows the directions along which you can move the handle. Some elbows can only move vertically (up/down) and some can only move horizontally (left/right).
4. Click-and-drag the elbow handle to a new location. Notice how the stream's segments are redrawn to adjust to the new location of the elbow.
5. Repeat with any other handle.
6. End the elbow editing session by clicking somewhere other than on an elbow handle.

The anchor point of an input stream (start point) and the anchor point of an output stream (end point) are also moveable by the procedure described above, as if they were elbows.

4.5 STREAM TAGS

4.5a Stream's Name Tag

As soon as a new stream in inserted in the process flowsheet, the program automatically assigns a new name that is displayed in a **name tag**. The name is always composed of a prefix and a number. The prefix is a section setting that defaults to 'S-' (for all sections), but can be

modified by the user (for more on sections, see 8.1 Sections & Branches). The number is chosen to be higher than a threshold value (also a section setting) set by default to 101, but can be modified by the user through the Section Properties Dialog: Auto-Numbering tab. The actual number picked is the first number available higher than the section's designated starting number that is not already used by any stream currently in the process. Users can change the tag name of the stream at any time.

▶ To edit the tag name of a stream...

1. Make sure you are in select mode (the button is pressed on the main toolbar).
2. Select the stream (move the mouse over the stream and click *once*).
3. From the context menu of the stream, select **Edit Tag Name** to bring up a dialog that displays the current name and allows you to type in a new name.
4. Type in a new name. When you are done editing the name, exit the dialog by clicking on **OK**.

The tag name of any stream should not exceed 15 characters in length and should be unique throughout the process file. After typing the new tag name and clicking on **OK** (or hitting **Enter**) the system will check if the new tag name provided is unique. If no conflict is detected, then the new tag name of the stream will be displayed; otherwise, you will be prompted to type yet another name or abort the whole renaming process and keep the original name.

The application uses a default font for displaying the tag names of all newly created streams. The font as well as several other characteristics of appearance of the stream in its entirety, are part of the stream's style (see 4.6 Stream Style). You can edit the style properties used for all present and future streams in a process (see 8.3 Default Style for Process Elements) or you can edit the style characteristics of just one stream through its Stream Style Dialog.

Even though you cannot move the tag with the mouse (by clicking-and-dragging it to another location), notice that the tag always follows the stream when the stream's segments are modified (relocated). The application automatically decides where to place the stream tag in relation to the stream's segments. By default, SuperPro Designer places the stream tag over the vertical segment closest to the start (source) of the stream, and if there's no such vertical segment (or the available vertical segments are too short to fit the tag), it places it under the first horizontal segment closest to the source of the stream.

Occasionally it may be desired to hide the name tag of a stream. The name tag visibility is also an element of the stream's style and can be turned on or off through the Stream Style Dialog: Stream Line Tab.

The user can provide his/her own preferences as to where stream tags should appear. There is a special set of attributes in a stream's style that addresses exactly this issue. These can be found in the Stream Style Dialog: Name Label Location Tab. If the name tag is turned off, this tab will not be part of the Stream Style Dialog.

Setting the tag location preference does not guarantee that the stream tag will appear where the preferences directly dictate as that choice may not be available for a particular stream. For instance, requesting that stream tags appear over the middle of vertical segments closest to the source may not be feasible for some streams as they may not have any vertical segments at all.

4.5b Stream's Information Tag

Besides the tag that displays the name of the stream, users can request to make visible another tag that can display customizable content. This second tag is called the **information tag** (or **info tag** for short). By default, all streams have their info tags turned off. The visibility of a stream's info tag is also part of the stream's style and can be turned on or off from the Stream Style Dialog: Stream Line Tab. The contents of the info tag can be a combination of the following stream properties:

1. Temperature
2. Pressure
3. Total Mass Flow
4. Total Volumetric Flow
5. Total Enthalpy
6. Specific Enthalpy
7. Heat Capacity

The units chosen are either the defaults (as set at the process level, see 8.4 Units of Measure (Physical Units Options)) or the user's overwrites as set at the stream's i/o simulation dialog.

You can dictate which combination of values you wish to view on the stream from the Stream Style Dialog: Information Tag Tab. Please note that if the info tag is turned off, this tab will not be part of the Stream Style Dialog. The info tag cannot be moved around using the mouse but it always follows the stream and it is drawn in a location decided by the application. Just like you can dictate your preference as to where you wish to see the name tag displayed, you can also express your preference as to where (relative to the stream's segments) you wish to have the info tag be displayed. This is specified in the Stream Style Dialog: Info Tag Location Tab.

4.6 STREAM STYLE

The style of a stream is a collection of attributes that dictate the stream's appearance on the flowsheet and on paper (when printed). These attributes are:

- The stream's line (thickness, style, color)
- The name tag's characteristics (visibility, font, color, frame line, etc.)
- The name tag's location preference (with respect to the stream's segments)
- The info tag's frame line (visibility, font, color, content, etc.)
- The info tag's location preference (with respect to the stream's segments)

When a new stream is created, the system displays the stream using the default stream style (see 8.3 Default Style for Process Elements). There are two sets of default stream styles: one for bulk streams and one for discrete streams. The choices for the default stream styles can be modified by selecting the **Edit ▸ Process Options ▸ Preferences ▸ Default Styles ▸ Bulk Streams** (for bulk streams) and **Edit ▸ Process Options ▸ Preferences ▸ Default Styles**

▸ **Discrete Streams** (for discrete streams) from the main menu (when nothing is selected). As a shortcut, you can pick the same options from the flowsheet's context menu.

If you wish to set a specific stream's attribute (e.g. its line color) to something other than the default color, then select the **Style ▸ Edit Style** option from the right-click (context) menu of that stream. From that moment forward, all of the stream's style attributes will stay fixed to your settings and will not follow the default settings (even if the default settings are modified). If later it is no longer desirable to have a stream's style be an exception, you can instruct the program to revert to the default style for all streams of that type. This is done by selecting the **Style ▸ Use Default** option from the context menu of the stream.

Oftentimes, after a user has tweaked a stream's style to his/her liking, he/she may wish to copy the entire style of that stream and apply it to several others. Instead of selecting **Style ▸ Edit Style** for each stream and manually set the styles to your liking, the application offers a great shortcut (see below):

▶ **To copy-and-apply a stream's style to others...**

1. Make sure you are in select mode (the button is pressed on the main toolbar).
2. Select the stream whose style you wish to copy (click *once* on its line)
3. Select **Style ▸ Pickup Style** from its context menu, or simply click on the button of the visual object toolbar (see 13.5 Visual Objects Toolbar).
4. Select the target stream(s) that you wish to acquire the same style. Select the first stream by clicking on it, then add more streams (if desired) by clicking on them while holding the **Shift** key down.
5. Select the **Style ▸ Apply Style** from the command menu of any of the target streams, or click on the button of the visual object toolbar (see 13.5 Visual Objects Toolbar).

4.7 BULK STREAMS

Bulk streams represent flow of bulk material (e.g. water, air, etc.). Bulk streams are only allowed to hook onto bulk ports of procedure icons (see 5.5 Unit Procedure Ports). The flowrate is specified and reported in the usual flowrate units (kg/h or L/h if the plant mode of operation is continuous and kg/batch or L/batch if the plant's mode is batch). The material can be in one or more liquid phases, solid or gaseous phase, but the application only distinguishes a vapor (gaseous) and a single liquid/solid phase (two phase system). Every component in the stream may distribute differently between the liquid/solid phase and the vapor phase. Each component's vapor fraction represents the percentage of that component that is considered to be in the vapor phase of the stream. The application may use a simple criterion (e.g. based on a component's normal boiling point and the stream's temperature) to determine if the component is in gaseous or liquid/solid state or it may use other more elaborate criteria. The criterion used throughput the process can be as one of the process defaults (see 8.12 Physical State Calculation Options) but it can also be overwritten for a given stream from the 'Physical State' tab of its i/o simulation dialog (for input streams, see 4.7d Stream Physical State Calculation Options; for intermediate and output streams, see 4.8 Discrete Streams).

4.7a Viewing and Editing the Simulation Data of Bulk Streams

Most properties of bulk input streams are provided by the user whereas for output and intermediate streams only the physical-state specifications are editable. The flowrate, composition, temperature and pressure of intermediate and output streams are determined by the simulation outcome. You can inspect the properties of any stream by bringing up its input/output (i/o) simulation dialog.

▶ **To display the i/o simulation dialog of a stream...**

1. Make sure you are in select mode (the button is pressed on the main toolbar).
2. Right-click on the stream to display its context menu; then select **Simulation Data**.

As a shortcut to the above procedure, you can bring up the i/o simulation dialog of a stream by simply double-clicking on it.

When viewing the composition table of an intermediate stream notice that only components with amounts above a set threshold are shown. The threshold below which a component is assumed to be practically zero and not shown on the table can be set from the .Physical Units Options Dialog.(zero flow threshold).

4.7b Composition & Related Properties of a Bulk Input Stream

Input streams represent material that is directly fed into the process. The user must initialize the amount, composition and state of the material as it enters the process.

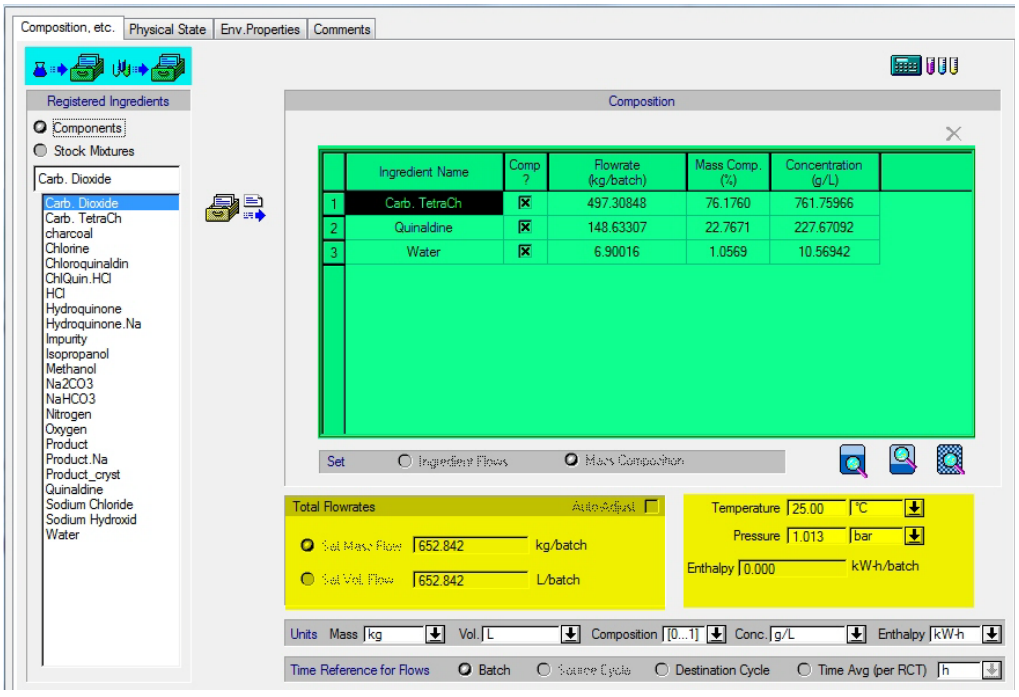


Figure 4.2: The 'Composition, etc.' tab for a bulk input stream.

You can set the above information by visiting the i/o simulation dialog for an input stream. The information is presented on the 'Composition, etc.' tab (Input Stream Dialog: Composition, etc.

Tab). As shown in Figure 4.2, this tab displays the state of an input stream as a whole (temperature, pressure, total flow - yellow fields in Figure 4.2) as well as component-specific information (mass flow, weight percent, concentration and perhaps extra-cellular fraction for each ingredient currently included in the stream - green fields in Figure 4.2). When a stream property is not editable (e.g., the enthalpy property), it is displayed in a grayed framed box. Notice that by clicking with the mouse inside such grayed frames, you cannot get into edit-mode and type new values in those fields. These properties are updated automatically by the application and are included on the dialog for display purposes only.

The user-editable stream properties in this tab are:

1. Temperature
2. Pressure
3. Composition

To specify the temperature or pressure of the stream simply click in the corresponding field and type a value. The composition of the stream, on the other hand, is specified in two steps:

(a) First, introduce all the ingredients (components and/or mixtures) that make up the stream. If you wish to introduce a component, then first click on the 'Components' button under the 'Ingredients' box on the left, to display the list of registered components. Then, select the desired component and click on the button (or simply double-click on the component's name). Notice that the table of ingredients (displayed on the right) will expand by one line (unless the ingredient is already there). The newly added ingredient may not appear last as the ingredients are sorted by their 'Local Name'. If you wish to introduce a stock mixture, first click on the 'Mixtures' button of the 'Ingredients' box to display all the registered stock mixtures, then click on the button.
If you wish to remove an ingredient already present in the composition table, select the ingredient in the table and click on the button.

(b) For each ingredient, specify its relative participation in the composition of the stream. There are two different ways this can be accomplished:
- Set the flowrate of each ingredient (this indirectly sets the total stream flowrate), or
- Set the total stream flowrate and the mass or mole percentage of each ingredient.
You can click on 'Set Ingredient Flows' or 'Set Mass Composition' (shown under the ingredient composition table) to dictate your preference.

The list of ingredients (pure components and stock mixtures) available to be included in the composition of an input stream include only those that have already been registered. If you don't find the ingredient needed, you must register them first through the Pure Component Registration Dialog or the Stock Mixture Registration Dialog. Instead of exiting the stream's initialization dialog and selecting ***Tasks ▸ Pure Components ▸ Register, Edit/View Properties...****, or* ***Tasks ▸ Stock Mixtures ▸ Register, Edit/View Properties...****,for convenience, two buttons allow a user to invoke either of the above interfaces without leaving the stream dialog (shown in Figure 4.2 above highlighted in blue). After visiting either of the aforementioned interface to add a component (or a mixture), upon return to the stream dialog, the component (or mixture) is readily available in the list of ingredient options and can be added in the composition list of the stream.*

For some simulations, tracking the activity level of a stream is important. For such cases, an Activity Reference component must have been selected (*see 3.1b Pure Component Registration*

Dialog). If that is the case, then another field is shown on the stream's 'Composition tab' (see Figure 4.3):.

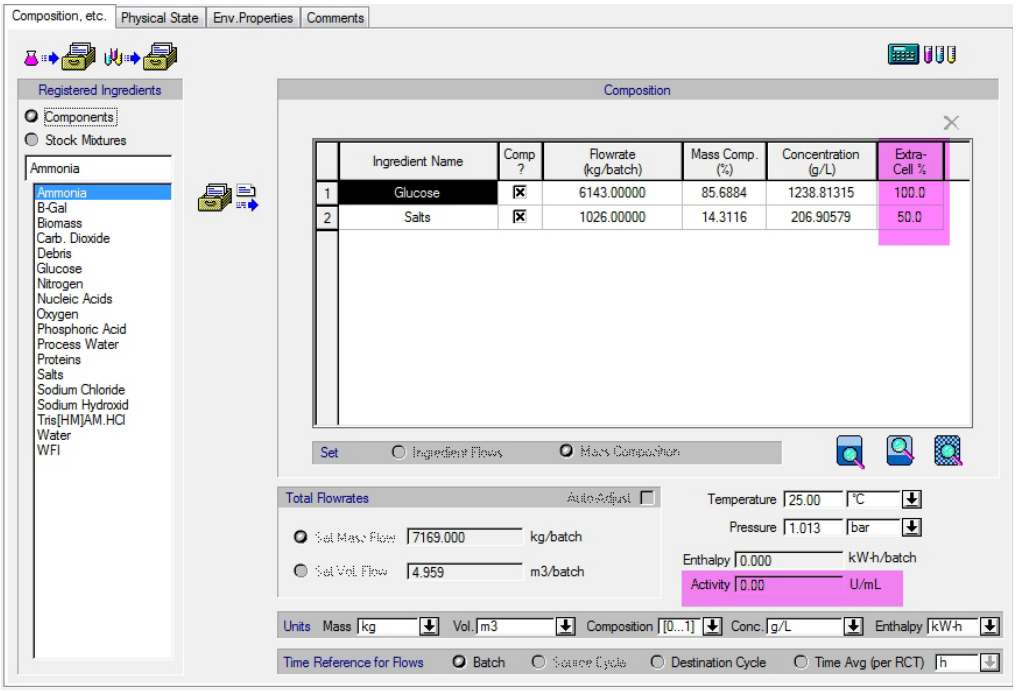


Figure 4.3: The 'Composition, etc.' tab for a bulk input stream with Activity and Extra-Cellular Column.

Please note that the 'Activity' value is always being calculated by the program (based on the presence of the 'Activity Ref. Component' in the composition of the stream, and therefore, the value will always be shown greyed out and will not be available for editing.

Also, if a 'Primary Biomass' component has been selected in the Component Registration dialog (see *3.1b Pure Component Registration Dialog*) along with a 'Water' component and a water content percentage, then the composition table for each stream has another column that displays the extra-cellular percentage of each component (see purple highlight in Figure 4.3). This percentage represents the portion of that component that can be found outside the "Primary Biomass" cell; the rest of that component is assumed to be part of the composition of the cells, and therefore, when an operation step diverts part (or all) of the biomass cells to a separate stream, it carries with it an amount of each component that is dictated by the intra-cellular percentage of that component. Please note that for process simulations that do not keep

track of intra- and extra- cellular presence of components (and therefore do not have a definition for the 'Primary Biomass' component, the above columns are not shown.

When setting the total stream flowrate and the ingredient percentages, you can choose to set either the total mass or volumetric flowrate (pick 'Set Total Mass Flow' or 'Set Total Vol Flow' in the 'Flowrates' box). When setting the flowrates of individual ingredients, you must always set the mass flow. The units for setting and viewing all of stream's properties are chosen based on the default settings for the process (see 8.4 Units of Measure (Physical Units Options)) but they can be customized for a given stream through this dialog as well. If you make a choice for units that is different from the default choice, the application will record your choice for that stream and use it every time you view the properties of that stream.

Sometimes users may not know the mass percentage of components in an input stream, but instead they may know the concentration of one (or more) components in the stream. Even though the stream's i/o dialog displays the concentration of each component directly on the composition table, it does not allow you to click-and-edit it directly. The main reason is that while the only restriction that exists when specifying individual mass percentages is that they all add up to 100%, concentrations on the other hand are related to each other and the stream's density and therefore cannot be all set independently of each other. SuperPro Designer offers a utility, the Target Concentration Calculator Dialog, that can assist the user in determining the stream's composition in order to meet certain concentration targets. You an invoke the Target Concentration Calculator Dialog by clicking on the button shown above the composition table.

If the conditions (temperature, pressure and composition) are such that two phases may exist, the composition tab shows the total composition (for both phases). If you wish to view the elemental (pure component) composition for the stream, you have three options:

1. Click on to view the component-based composition of what the application considers as the liquid/solid phase of the stream.
2. Click on to view the component-based composition of what the application considers as the gaseous phase of the stream.
3. Click on to view the component-based composition for the entire stream (both phases).

Note that the application determines the state of each component based on its physical state options settings (through the Bulk Input Stream Dialog: Physical State Tab). The distribution of each component to the liquid/solid or gaseous state also affects the density of the stream and therefore the dependency between the mass flowrate and volumetric flowrate of the stream.

When the plant mode of operation is set to batch (see 8.14d Process Operating Mode: Batch vs. Continuous), stream flows can be displayed on a per-batch, per-destination-cycle (if there's a destination procedure), per-source-cycle (if there's a source procedure) basis or on a per-time average Recipe Cycle Time basis. When the overall mode of operation is set to continuous, all stream flowrates are displayed on a per-time-average basis (either second, minute, hour, day or week). However, there is one exception: streams that appear as inputs to a unit procedure set to operate in batch mode (e.g. a batch distillation procedure, or a batch filtration operation), will display their flows in amounts/cycle (of the destination procedure) even in continuous processes.

Sometimes it is convenient to initialize the contents of an input stream such that they match exactly the contents of another (input, output or intermediate) stream.

▶ **To initialize an input stream based on the composition of another stream...**

1. Make sure you are in select mode (the button is pressed on the main toolbar).
2. Select **Copy Contents** from the source stream's context menu.
3. Locate the input stream that you wish to be initialized, and select **Paste Contents of <source-stream-name>**.

*The command **Paste Contents of <Source-Stream-Name>** is only available as part of the context menu of input streams only and while the source stream has not been deleted.*

THE INPUT STREAM'S AUTO-ADJUSTABLE FLAG

Some input streams may need to have their total flowrate indirectly set by the application (as part of the simulation calculations) in order to satisfy some other requirement. For example, consider a input stream providing material for a wash operation in a chromatography column. The amount of wash is typically dictated by the user on the operation's i/o simulation dialog and it is typically expressed in 'Column or Bed Volumes', therefore the actual amount (in L/h or L/batch) will not be known until the M&E balances are executed. Also, consider a simply 'Charge' operation where the user has dictated the amount to be charged on the i/o simulation dialog of the operation. Once again, the amount of material that needs to be carried in by the stream servicing that charge needs to be set indirectly to match the user's choice. For simple circumstances like those mentioned, the application automatically checks the 'Auto-Adjustable' flag of the input stream associated with the operation. There are also other, more involved circumstances where the back-propagation calculation mechanism may require certain input streams to have their 'auto-adjustable' flag set (see 8.14i Back-Propagation: Sources (Initiators) & Sinks (Terminals)). For those circumstances, the user must set the flag him/herself.

When the application itself has turned the 'auto-adjustable' flag on, the 'Auto-Adjustable' check box is shown as checked and the setting is disabled; in other words, the user cannot un-check it. Only when the conditions that require this setting are removed (e.g. the operation that is serviced by that stream is deleted, or the user assigns a different stream to carry out the operation - through its i/o dialog) then the flag will be removed and the setting may become editable once again.

When the 'auto-adjustable' flag of an input stream is set (checked), then the application will set the total flowrate amount to '100 kg/batch' (or '100 kg/h' if the plant's operating mode is continuous) and it will prevent the user from editing the value. The composition must only be specified by providing the mass percentage of each ingredient (but not their flowrate - this mode is also disabled).

4.7c Composition & Related Properties of Intermediate and Output Streams

Unlike input streams, the composition, temperature and pressure of intermediate and output streams is calculated by the outcome of the M&E balances, therefore, when displaying the i/o simulation dialog for such streams, the information presented on the 'Composition, etc.' tab (Bulk Intermediate/Output Stream Dialog: Composition, etc Tab) is for viewing only. Notice that all the fields used to display the mass flow, volumetric flow, temperature, pressure and

enthalpy are greyed out and you cannot click to edit them (see Figure 4.5).

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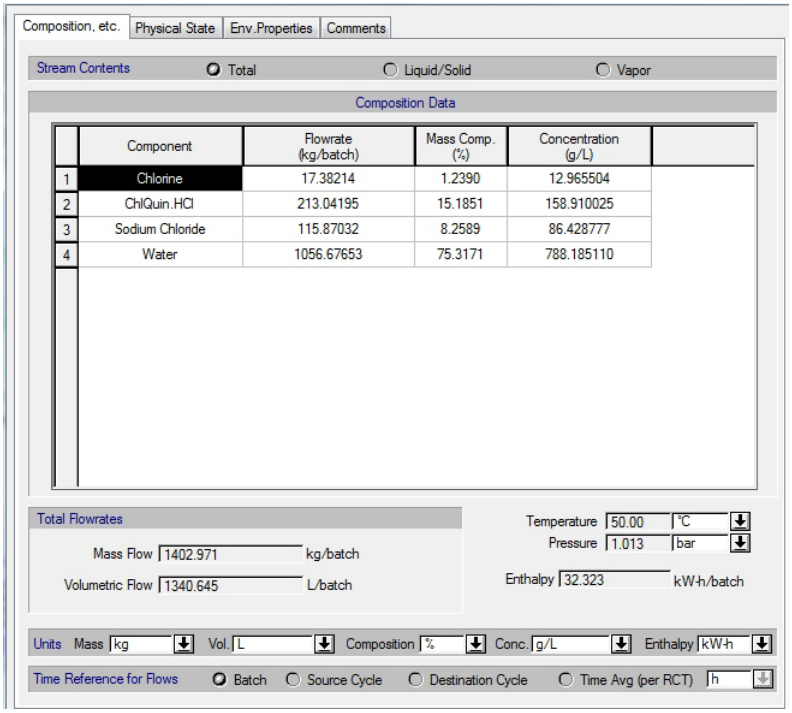


Figure 4.4: The 'Composition, etc.' tab for a bulk intermediate or output stream.

The only settings that can be changed are the viewing preferences. At the top of the dialog, you may choose to:

(a) View the composition of the entire stream

(b) View the composition of only the portion of the stream that the application perceives as the liquid/solid phase, at the current stream conditions and using the physical state criteria for the stream, see 4.7d Stream Physical State Calculation Options.

(c) View the composition of only the portion of the stream that the application perceives as the vapor phase, at the current stream conditions and using the physical state criteria for the stream, see 4.7d Stream Physical State Calculation Options.

After the solution of the M&E balances, intermediate and output streams are assigned enthalpy values which are calculated ***based on the specific PS calculation options of their associated procedures.*** *These enthalpy values will be respected by the streams at the expense of respecting a given temperature. In practice, this means that if the PS calculations options of an intermediate or output stream are different than the respective options of their associated procedures, deviations in the displayed temperature may be observed. This respect-enthalpy behavior, however, is necessary in order to eliminate the generation (or loss) of enthalpy content in a process that would otherwise occur because of the discontinuity between PS calculation options between a stream and its associated procedure.*

Near the bottom of the dialog, you may pick the units of choice for the presentation of mass & volume quantities, concentrations, composition percentages and flow time reference. When the

streams is first displayed the defaults as set for the entire process are used (see 8.4 Units of Measure (Physical Units Options)), but users may overwrite the defaults for any given stream next time the stream's i/o simulation dialog is presented.

The last viewing choice that can be made is the time reference for the flow values. The exact choices depend on:

(a) The operating mode of the process (see 8.14d Process Operating Mode: Batch vs. Continuous).

(b) The operating mode of the source procedure (if it exists) and the destination procedure (if it exists). For more on how to view and/or change the procedure's operating mode, see 5.2 Unit Procedure Operating Mode.

It should be noted that if the user has specified an "Activity Reference" component and a "Primary Biomass" component in the , then the there are "Composition, etc." tab of an intermediate (or output) streams appears as shown in Figure 4.5 below..

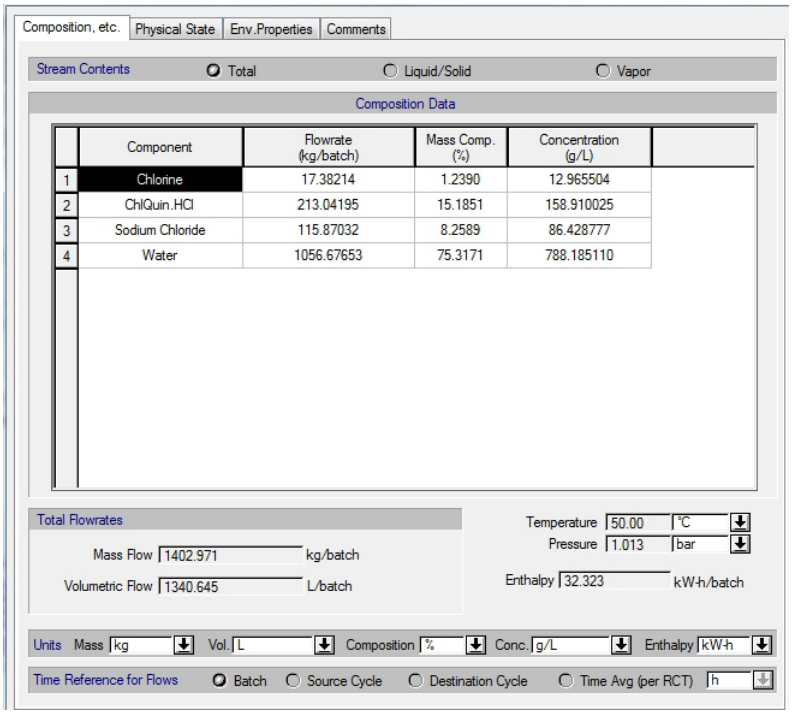


Figure 4.5: The 'Composition, etc.' tab for a bulk intermediate or output stream with activity and extra-cellular information displayed

4.7d Stream Physical State Calculation Options

Material in streams is considered to be in either vapor or liquid/solid state. For each bulk stream, SuperPro Designer calculates the Physical State (PS) of each component by either a simplified component-specific set of criteria (i.e., the Shortcut PS Toolbox) or by an elaborate

VLE Model (i.e., the Rigorous PS Toolbox). A detailed description of the physical state calculation options is given in 8.12 Physical State Calculation Options.

*The PS of a stream is indicated by the vapor fractions percentages of its components. The **component vapor fraction** (i.e., the moles of the component in the vapor phase divided by the total moles of the component) must not be confused with the **molar fraction of the component in the vapor phase** (i.e., the moles of the component in the vapor phase, divided by the total moles of all components in the vapor phase).*

In principle, the PS calculation options of streams have only an indirect impact on the simulation outputs through the calculation of their enthalpy content. In other words, the overall energy balance around a procedure will calculate the enthalpy content of the input streams to that procedure based on the PS calculation options of these streams.

By default, every bulk Input Stream in the process is initialized with the Shortcut PS calculation toolbox while every Intermediate/Output stream is assigned with the PS Toolbox of its associated unit procedure. It is possible to deviate from the default settings for the calculation of the physical state of streams in one of the following ways:

1. *Modify the assigned PS Toolbox*. While the Shortcut PS Toolbox offers a quick way to determine the physical state of a stream, the Rigorous PS Toolbox calculates the distribution of components in the vapor and liquid/solid phase in a more realistic manner. As a rule of thumb, the Shortcut Toolbox should be used when the accuracy of physical state calculations is not a primary concern or when no change of phase occurs in the process.
2. *Modify the options of the assigned toolbox.* For example, it may be necessary to change the Shortcut PS Toolbox V/L split criterion of a component (e.g., ammonia) from the default *Normal Boiling Point* to *Liquid/Solid Only* as it may be known that, at the conditions of the stream, all ammonia present in the mixture is dissolved in the liquid phase. On the other hand, given a stream that uses the Rigorous PS Toolbox (e.g. a mixture of hydrocarbons for which the binary interaction coefficients are readily available), an *EOS model* (e.g., the Peng-Robinson or the SRK) is best suited than the default *Raoult's law.*

CUSTOMIZING THE PHYSICAL STATE CALCULATION OPTIONS OF STREAMS

▶ How to select between the Shortcut or the Rigorous Toolbox...

1. While in select mode (i.e., the button is pressed on the main toolbar), double-click on the specific stream whose Physical State calculation options you wish to change. Alternatively, right-click in the stream and select **Simulation Data.**
2. Visit the Physical State Tab.
3. Check the Overwrite checkbox in the Physical State (PS) Calculation Options frame (see Figure 4.6).
4. Select between the Shortcut or Rigorous PS Toolbox option.

Figure 4.6: Selection between the Shortcut and the Rigorous Toolbox for the calculation of the stream's physical state.

For Intermediate/Output Streams, the PS toolbox selection and options are, by default, imposed by their associated procedure. This means that any change to the procedure's PS calculation options is automatically propagated to the stream. Checking the Overwrite option allows the stream to differentiate its behavior and adopt a different set of PS calculation options from its associated procedure. As a consequence, any change to the PS calculation options of the procedure will not be propagated to the stream.

For Input Streams, the PS toolbox options (but not the PS Toolbox selection) are, by default, imposed (inherited) by the process file (i.e., any change to the process file's PS Toolbox Options is automatically propagated to the stream). Checking the Overwrite option allows the stream to differentiate its behavior and adopt a different set of PS calculation options from the process file. As a consequence, any change to the PS calculation options of the process file will not be propagated to the stream.

▶ How to customize the Shortcut Toolbox options...

1. While in select mode, double-click on the stream whose options you wish to change or right-click in the stream and select **Simulation Data.**
2. Visit the Physical State tab.
3. Check the Overwrite checkbox in the Physical State (PS) Calculation Options frame.
4. Make sure the Shortcut Toolbox option is selected.
5. Check the **Custom?** checkbox for the specific component you wish to change the V/L split criterion (see Figure 4.7).
6. From the V/L Split Criterion drop-down list, select the criterion of choice (see 8.12a The Shortcut Physical State Calculation Toolbox for more details).

You can apply the *customized* V/L split criterion of a component to the rest of the components in the stream by selecting that component and then pressing the button.

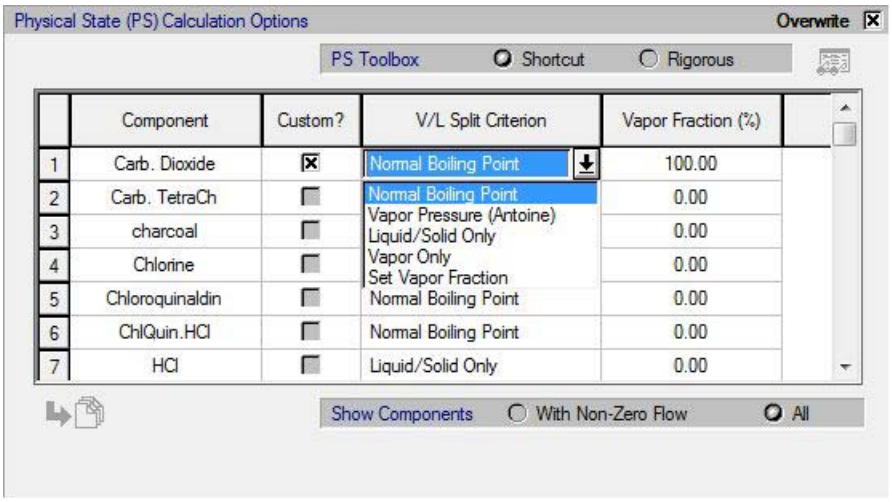


Figure 4.7: The Physical State calculation options tab for a bulk stream.

By alternating between the Show Components With Non-Zero Flow and All options, you request to view (or omit) the components that have zero flow, and therefore do not actually affect the composition of a stream.

▶ How to customize the Rigorous Toolbox options...

1. While in select mode (the button is pressed on the main toolbar), double-click on the specific stream whose options you wish to change or right-click in the stream and select **Simulation Data.**
2. Visit the Physical State tab.
3. Check the Overwrite checkbox in the Physical State (PS) Calculation Options frame.
4. Make sure the Rigorous Toolbox option is selected.
5. Click on the Edit Rigorous Toolbox Options button .
6. In the Rig. Toolbox dialogue that appears (Figure 4.8), specify the desired VLE model from the K-value calculation model drop-down list (see 8.12b The Rigorous Physical State Calculation Toolbox for more details).

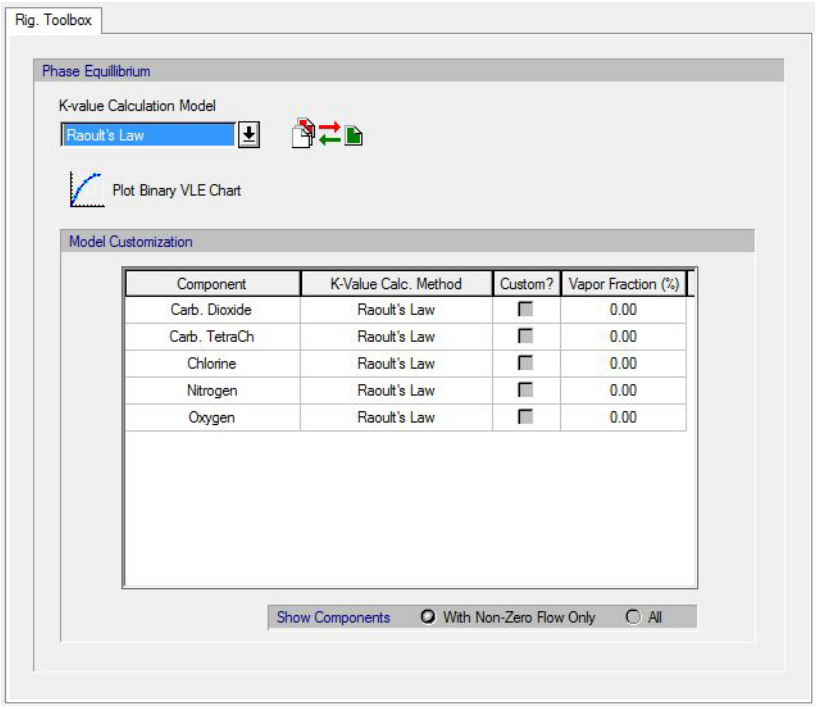


Figure 4.8: The Rigorous Toolbox dialog.

Streams that are outputs of Rigorous toolbox-only procedures have their PS determined by the procedure itself. The PS calculation options of such streams cannot be overwritten (see Rigorous Toolbox-Only Unit Procedures).

4.7e Stream Density Calculation Options

For each bulk stream, SuperPro Designer calculates the individual densities of the liquid/solid and vapor phase (see 8.13 Density Calculation Options) as well as the total density of the stream. By default, every stream in the process is initialized with the density calculation options of the process file (unit procedures do not keep a set of default options for density calculations) and any change to the options of the process file will be propagated to the stream. It is possible to deviate from the default settings for the calculation of density in one of the following ways:

1. Modify the liquid/solid density calculation options
2. Modify the vapor density calculation options

When the Overwrite check box is checked, the density calculation options of the stream become independent of the respective options of the process file. As a consequence, possible changes to the density calculation options of the process file will not be propagated to the stream.

CUSTOMIZING THE DENSITY CALCULATION OPTIONS OF STREAMS

▶ How to overwrite the Density Calculation Options...

1. While in select mode, double-click on the specific stream whose physical options you wish to change.
2. Visit the Physical State Options Tab.
3. Check the respective Overwrite checkbox for the Liquid/Solid or Vapor Density (Figure 4.9).
4. Make the desired changes regarding user-set density values, volumetric coefficients, etc.

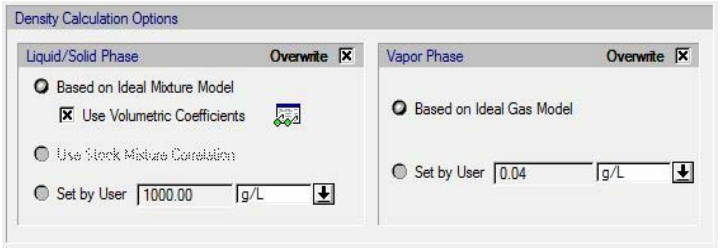


Figure 4.9: The input stream's density options

The density options for a bulk input stream are identical to the options available for intermediate and output streams unless the input stream's composition is just a single ingredient that happens to be a stock mixture. In that case there is one extra choice for the liquid/solid density model: 'Use Stock Mixture's Density Correlation'. If chosen, then the application will calculate the density of the stream with the density options of the stock mixture (see Stock Mixture: Composition & Density).

4.7f Environmental Properties of Bulk Streams

All environmental properties of the stream are always calculated based on the composition of the stream and the environmental contribution factors of the components that are present in the stream (see 'Pure Component: Aqueous Properties' on page 3-15). They are presented (for viewing only) on the Bulk Stream Dialog: Env. Properties tab.

This tab may not be shown (for all streams). Since environmental assessment properties are only pertinent to users whose main focus lies in that area, and not to all other users, there is an option to hide all such information (for simplicity) from all other users. The option is part of the dialog that appears when selecting **Preferences ▸ Miscellaneous...** *from the flowsheet's context (right-click) menu. Please note that when this tab is not shown on streams, the "Aqueous Prop" tab of a pure component's definition dialog is not shown either.*

The dialog displays the concentrations (in mg/L) and daily throughputs (kg/day) of the following environmental properties:

- Total Organic Carbon (TOC)
- Total Phosphorous (TP)
- Total Kjeldahl Nitrogen (TKN)
- Ammonia Nitrogen (NH3)

- Calcium Carbonate (CaCO3)
- Nitrate/Nitrite Nitrogen (NO3-NO2)
- Chemical Oxygen Demand (COD)
- Theoretical Oxygen Demand (ThOD)
- Ultimate Biochemical Oxygen Demand (BODu)
- 5-Day Biochemical Oxygen Demand (BOD5)
- Total Solids (TS)
- Total Suspended Solids (TSS)
- Volatile Suspended Solids (VSS)
- Degradable Volatile Suspended Solids (DVSS)
- Total Dissolved Solids (TDS)
- Volatile Dissolved Solids (VDS)
- Degradable Volatile Dissolved Solids (DVDS)

4.8 DISCRETE STREAMS

Discrete streams represent the flow of discrete entities (e.g. a “2L Plastic Bottle”). Discrete streams are only allowed to connect to discrete (input or output) ports of procedure icons. Their flowrate is measured in Entities/h (for processes in continuous mode) or Entities/batch (for processes in batch mode). Each discrete stream can only carry one type of entity.

4.8a Entity & Entity Properties

An entity is any matter that can be carried by a stream in discrete quantities (in contrast to bulk material that can be carried by a stream in any quantity). Examples of entities can be: a “1L Empty Bottle”, a “12oz Filled Can”, a “Mid-Size Box”, an “Empty Six-Pack”, etc. Users may engage such discrete entities to describe the contents of (discrete) streams. For example, in order to describe the contents of a line with soon-to-be-filled empty 12oz bottles, we need to introduce the entity of “Empty 12oz Bottle”. In order to define an entity you need to provide the following attributes:

1. Name: A string of up to 31 characters; it must be unique amongst all entities defined in a process.
2. Bulk Amount per Entity: Allows the program to convert the bulk equivalent mass into discrete entities; it can be either in mass or volume units.
3. Purchase Price: used when this entity is being sold (on a ‘Revenue’ output stream)
4. Selling Price: used when this entity is being purchased (on a ‘Raw Material’ input stream)

Unlike pure components or stock mixtures, entities are not formally registered in a process through a central interface. Instead, they are defined at the spot where they are needed. There are only two locations where entities can be defined:

(a) As part of a discrete input stream that describes the feed of discrete entities into the process (such as the line of empty 12oz bottles mentioned above). In that case, the four essential properties of the entity (name, bulk amount per entity, selling and purchase price) are directly provided on the Discrete Input Stream Dialog: Entity Tab.

(b) As part of an operation that produces an entity (e.g. a filling operation, or a packaging operation, etc.). To continue with the example of empty 12oz bottles mentioned previously, once those bottles are fed into a filling operation, on the other side, we need to have an output of "Filled 12oz Bottles". In that case, users get the chance to define this new entity as part of the operation that will combine one (previously defined) entity and perhaps some bulk material. Other times, an operation may use (consume) all bulk streams but generate (output) a discrete entit: e.g. a molding operation or a tableting operation. Other times the operation may consume one (or more) discrete lines and produce (output) a new entity line: e.g. a labelling operation, an assembly operation, etc. In all such cases, the four essential properties of the new entity that is being produced by the operation are defined as part of the 'Oper. Cond's' tab of the operation that produces it.

The properties of a discrete entity will be displayed on every discrete stream that carries it but can only be changed from the interface that introduces the entity: either the i/o simulation dialog of the discrete input stream where the entity first enters the process, or the i/o simulation dialog of the operation that is responsible for first manufacturing the entity.

4.8b Discrete Input Streams

Discrete input streams represent material that is being fed into a process in the form of such countable (discrete) entities. Even though users must specify the flow of such streams in terms of entities/h or entities/batch, they must still have to describe to the application the composition of the bulk material that makes up the entity. For example, if the discrete input stream is to represent the flow of empty (but soon to be filled) aluminum 12oz cans, you can describe the composition of the bulk material as 100% Aluminum; if the input stream represents the flow of empty (to be filled) vials, you can specify the composition of the bulk material as 100% glass. The information about the composition of the bulk material may be used if the entity is ever processed through an operation that converts it back to the bulk material that it is made. For example, consider a grinding operation or shredding operation, or even the generic 'discrete-to-bulk' operation. Please note that the composition of the bulk material that each entity is constructed is provided in the second tab (the Input Stream Dialog: Composition, etc. Tab). The first tab of the stream's i/o dialog is dedicated to defining the entity that is carried by the stream, and thus it provides for fields that will capture the four essential properties of the entity carried

by the stream (see Figure 4.10).

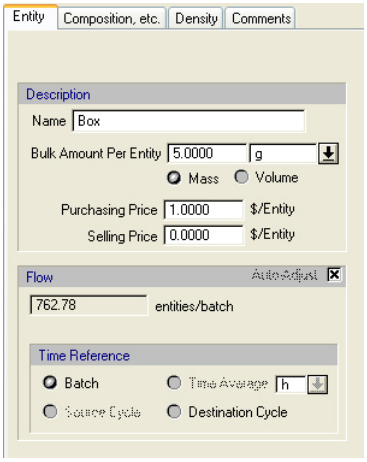


Figure 4.10: The 'Entity' tab (entity definition) on a discrete input stream.

If the 'auto-adjust' flag is checked on a discrete input stream, the entity flow of the stream will be determined by the application. For example, in a bottle-filling operation, once the bulk material comes into the bottling step (as the bulk input) and the user specifies the amount of bulk material to be added per bottle (as part of the operation's i/o dialog), then the other input of the operation (carrying empty bottles) will have it entity flow automatically adjusted so that all the bulk material is properly accommodated.

DENSITY SPECIFICATION OF DISCRETE INPUT STREAMS

The density-related information of discrete input streams, pertains to the density of the bulk material that makes up each entity. It will be used by the application only if the 'bulk amount per entity' specification for the entity is in volume units. If that is the case, then in order for the application to determine the entity flow for the stream, it will need to convert the bulk mass into volume and then use the 'bulk amount per entity' factor to determine the number of entities carried by the stream. The density of the bulk material can either be provided by the user or be calculated by the application using the volumetric contribution model. This is specified in the Discrete Stream Dialog: Density Tab.

4.8c Viewing and Editing the Simulation Data of Discrete Streams

You can display the i/o simulation dialog of discrete streams in just the same way as for bulk streams (see 4.7a Viewing and Editing the Simulation Data of Bulk Streams). Some of the variables that characterize bulk streams are not present on discrete streams (e.g. temperature, pressure, enthalpy). Furthermore, discrete streams always present information about the entity that is being carried by the stream (name, bulk amount per entity, etc.). Users are allowed to edit the entity definition parameters, the entity flow as well as the bulk material composition on discrete input streams. Discrete intermediate and output streams have all such information filled-in by the mass and energy balance calculations. Consequently, all such date are only presented on the i/o simulation dialog for display only.

4.9 AUTO-INITIALIZATION OF INPUT STREAMS

Typically the state of input streams (bulk or discrete) is initialized by the user through the i/o simulation dialog (the Bulk Input Stream Dialog or the Discrete Input Stream Dialog). From that interface users provide the temperature, pressure, flow and composition of the stream. You may also copy the contents of one stream and paste them to an input stream (see 'To initialize an input stream based on the composition of another stream...' on page 4-15). Sometimes, it may be convenient to have the application perform such an action automatically. Typically this need arises when users are faced with a very long process that may be easier to model (simulate) if broken apart into smaller fragments. Each fragment may represent the production of an intermediate chemical that is later used as a feed in the main process; or the intermediate may itself be used as a feed for another fragment process that produces another intermediate. Either way, when modeling such complex processes whose simulation models span across process files, users will find it convenient to have the application initialize the contents of an input stream based on a source stream that may not even reside in the same process file.

▶ To auto-initialize an input stream...

1. Make sure you are in select mode (the button is pressed on the main toolbar).
2. Select **Initialization Options** from the input stream's context menu. This will bring up the Input Stream Initialization Options Dialog.
3. From the ensuing Input Stream Initialization Options Dialog choose 'Auto-initialize from Other Stream'. Specify which variables of the input stream you wish to be copied from the source stream (temperature, pressure, composition, flow).
4. Schedule when you wish to have the application perform the auto-initialization. Typically, it is expected that the auto-initialization is performed before the M&E balances are executed. However, if the source stream is in a process file that doesn't change any more, you may want to perform the initialization manually once and never again (to save time).

▶ Viewing and Editing Auto-Initilization Links

The user may view and/or edit the auto-initialization links of all input streams and equipment contents from a central location in SuperPro. For more information on this feature, see Auto-Initialization Links.

4.10 CLASSIFICATION OF INPUT AND OUTPUT STREAMS

As mentioned in 4.1 Types of Streams, streams can be considered as input, output or intermediate (based on their source and destination procedures) and bulk or discrete (based on the type of material they carry). The above classification of streams is based on the inherent nature and cannot be explicitly set by the user. There is one more classification category that can be assigned to streams based on how they are treated from the economic standpoint. This set of options only apply to input or output streams (not intermediates) and even though the application will make some assumptions and automatically apply one of the available options

to some input and/or output streams, users may overwrite the settings and apply their own choice using the Stream Classification Dialog interface (see Figure 4.11)

The choices available depend on whether the stream is an input or an output.

The economic classification choices for input streams are:

(a) Raw Material,

(b) Revenue or

(c) Cleaning Agent,

whereas the choices for an output stream are:

(a) Revenue,

(b) Credit,

(c) Solid Waste,

(d) Aqueous Waste,

(e) Organic Waste or

(f) Emission

Note that sometimes (c), (d), (e) or (f) categories may be referred to collectively as 'Waste'. Also, an output stream may also be tagged as 'Hazardous' by the user. This tagging simply instructs the application to report the contents of that stream under a dedicated category in the environment impact report, but it does not directly affect the economic evaluation.

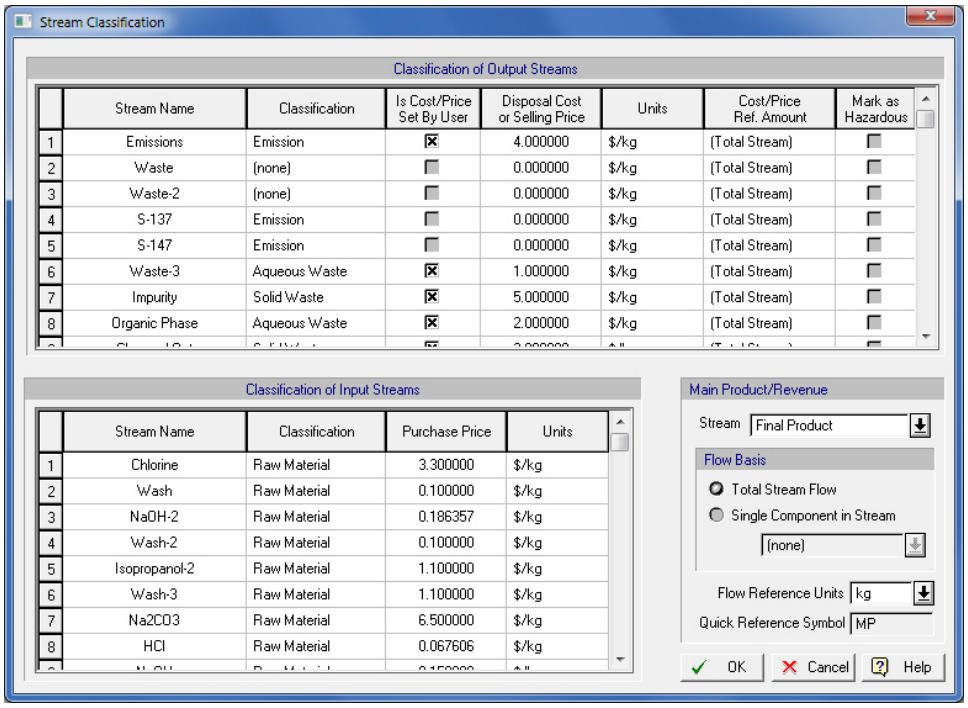


Figure 4.11: The stream classification interface.

RAW MATERIAL, REVENUE AND CREDIT STREAMS

All input streams are by default classified as 'Raw Material' streams. The implication is that material present on such streams is assumed to be consumed by the process directly towards the manufacturing of the main product. Even though materials as a resource can be consumed by the process indirectly through several other uses (e.g. as 'Cleaning Agents', or 'Heat Transfer Agents', see 6.5 Materials) the lion's share of consumption is typically as 'Raw Materials'. The cost of raw materials will be reported in the Economic Evaluation Report (EER) and the Itemized Cost Report (ICR). Streams tagged as 'Raw Material' will contribute to the tracking of materials assumed to consumed as 'Raw Materials' by the process. The consumption of raw materials during the span of a single or multiple batches can be presented in charts and tables (see 6.6 Material Charts & Tables).

Even though the amounts of material consumed by the process as 'Raw Material' is tallied up based on individual ingredient flows (as components or mixtures) on input streams tagged as 'Raw Materials', the contribution to cost is always tallied up on a stream basis, using the stream's purchase price (and not the price of ingredients directly). The price of ingredients (weighed by their relative mass fractions) will be used by the program to suggest a purchase price for the input stream but users may overwrite the price with their own value in the Stream Classification Dialog.

Both input and output streams can be classified as Revenue streams. A revenue stream is any stream that generates income. Typically, a revenue stream is an output stream that can be sold. Sometimes revenue streams are also called product streams. There may be several revenue (or product) output streams in a process. It may appear as odd, at first, to allow input streams to be tagged as 'Revenue' streams. The only reason this is allowed is to accommodate waste treatment facilities which usually charge their clients (and generate income) on a per-gal (or per-kg) basis of material that is being treated (and therefore is the main input to the waste treatment process). The selling price of bulk product streams is either estimated by the system (based on the selling prices of each ingredient and weighed by their mass fractions) or specified by the selling price of a specific ingredient in the stream (by selecting the ingredient fromthe 'Cost/Price Ref. Amount' column), but they can also be overwritten and set directly by the user on a per-mass or per-volume basis. To set the selling price of a stream, simply click on the 'Set by User' box displayed at the row that corresponds to that stream and then click in the 'Selling Price' cell and type in the desired value. The selling price of discrete product streams is set at the interface where the entity was introduced (most likely the i/o simulation dialog of the operation that produced it) and cannot be overwritten from the Stream Classification Dialog interface.

Finally, output streams can be classified as credit streams. These streams are basically revenue streams (as they can be sold at a fixed selling price) but the user has opted to treat revenues from such streams as credit against the operating cost of the process rather than an added revenue item in the proceeds coming from this process. The selling price of credit streams is set in the same way as revenue streams.

CLEANING AGENT STREAMS

Input streams can be classified as 'Cleaning Agent' streams if their intended use is not as part of the process chemistry but simply to clean equipment interiors. It is very common to use materials such as pre-made buffers or other stock mixtures to clean the interior of process vessels, chromatography columns, etc. Tagging such streams as 'Cleaning Agents' allows the

program to tally up their associated cost in a category separate from 'Raw Materials' in order to provide better insight.

WASTE STREAMS

The cost associated with waste treatment and disposal of material that leaves processes has skyrocketed in recent years due to increasingly stricter environmental regulations. Also, new regulations from the EPA (or similar organizations in other countries) require the tracking of the fate of certain chemicals in every process as well as the reporting of releases of offensive chemicals into the environment. SuperPro Designer provides several tools that help engineers to better understand the environmental impact of their process. It all starts with tagging the output streams of the process as 'Emissions' or one of three types of waste (Aqueous, Organic, or Solid). Waste, in this context, is considered any stream that has a deleterious effect on the environment and possibly carries a price tag for treatment or disposal. Emission, on the other hand, is considered any release vent to the atmosphere and may potentially include hazardous and/or regulated chemicals.

Only output streams can be tagged as wastes (or emissions). The waste treatment/disposal cost associated with a stream is calculated by the application based on their waste treatment/disposal cost of each component in its composition weighed by their mass fractions but it can be overwritten by the user. To specify your own unit cost, simply click on the 'Set by User' box on the row that represents the output stream, and then click in the price cell and type your own value. The unit price can be provided on a per-mass or per-volume basis. The unit price as well as the total cost for waster treatment and disposal are reported in the Itemized Cost Report (ICR) and Economic Evaluation Report (EER).

HAZARDOUS STREAMS

Some components can be marked by the user as hazardous in the Pure Component Properties Dialog: Pollutant Categories tab. If such components are present in an output stream at a concentration level higher than their hazardous threshold (another environmental component property) they automatically trigger the tagging of that stream as hazardous. Furthermore, you may decide to explicitly tag output streams as hazardous (if so desired). This can be done through the Classification of Input and Output Streams dialog. Any streams classified as hazardous will be listed in the hazardous stream section of the Environmental Impact Report (EIR). Marking a stream as hazardous incurs no further penalty on the economics of the project.

MAIN PRODUCT/REVENUE RATE STREAM

As mentioned above, there may be several output streams that can be tagged as 'Revenue' (or product) streams, all of them bringing income to the process as they have a positive selling price. However, in most cases, processes are built to manufacture a specific product and therefore, the revenues are expected to come mainly from the sale of that product. The Classification of Input and Output Streams dialog allows you to designate one of the previously tagged 'Revenue Streams' as the 'Main Product' ('MP') or 'Main Revenue' stream (see also 9.3q Main Product/Revenue Rate). If such a choice is made, then the proceeds from that stream are reported on a special line in the executive summary portion of the Economic Evaluation Report (EER) and the Executive Summary Dialog itself. Furthermore, the flowrate associated with that stream (on a total basis, or on a per-user-selected component basis) will be used to:

- Convert the annual operating cost to unit production cost.
- Report the size (or throughput) of the process and perform scale-up/down calculations.

If you wish to use different streams as the basis for either one of the two reference flows mentioned above, you can do so using the Rate Reference Flows Dialog (see below).

RATE REFERENCE FLOWS

The main product stream (as selected from the Stream Classification Dialog) is used to report the revenues associated with the 'main' product of the process, but also its flowrate is used as the reference basis to generate the unit product cost and to report the size (or throughput) of the process. Typically that is the case for most processes. However, sometimes users may find it more convenient to report the unit production cost using as flow reference not the main product rate but perhaps some other flowrate (it could be the amount of product in the output of the main reactor or fermentor). If you wish to choose a different stream to be used as a basis for either the unit product cost calculation or the size of the process, then select **Tasks ▸ Rate Reference Flows** from the application's main menu to present the Rate Reference Flows Dialog. From this interface you can make a different designation on what the program should use for the unit production reference flow (UPRF) and/or for the size (or throughput) reporting. Please note that for these assignments you are not restricted to use only revenue output streams, but you can pick any stream of the process (input, intermediate or output, revenue or non-revenue). For more on rate reference flows, see also 9.3r Unit Reference Rate (or Flow).

5 PROCEDURES & OPERATIONS

Building a process requires putting together all the processing steps that are necessary to carry out the full recipe. Each such process step is depicted on the workspace of SuperPro Designer's process flowsheet as an icon or more precisely a unit procedure icon (see 5.1 What Is a Unit Procedure?). The icon stands for a set of one or more elementary transformations (unit operations) (see 5.9 What Is a Unit Operation?) that are presumed to take place inside the same hosting equipment resource. Material is supposed to flow from one procedure to another via process streams. Sometimes material enters a process as a direct input to a unit procedure; sometimes material exits the process as a direct output from a a unit procedure.

As mentioned in 'Batch vs. Continuous Procedures' on page 8-31, SuperPro Designer can be used to simulate batch, continuous as well as mixed mode processes (partly batch, partly continuous). The intelligent behavior of unit procedures as simulation agents in a continuous or batch mode environment is a unique aspect of SuperPro Designer as a simulation engine and it is what makes this software unique amongst other simulation tools.

5.1 WHAT IS A UNIT PROCEDURE?

A **unit procedure** (aka a procedure) in the context of a SuperPro Designer simulation is defined as a sequence of actions representing the most elementary physico-chemical transformations supported by the software all assumed to take place inside the same equipment resource. Each such action is represented by a unit operation as described in more detail in 5.9 What Is a Unit Operation?.

▶ To Add a New Unit Procedure...

1. Make sure you are in select mode (the button is pressed on the main toolbar).
2. Select the unit procedure's type from the **Unit Procedures** submenu. Notice that the mouse pointer will change to:
   : The 'Add Unit Procedure' mouse pointer.
3. Click in an unoccupied area of the flowsheet. The unit procedure's icon will be inserted such that its center coincides with your last mouse click.

5.1a The Unit Procedure's Context (or Command) Menu

If you move your mouse pointer over a procedure it will turn into:

: The 'Command Menu' (or 'Context Menu') mouse pointer

indicating that if you right-clicked over that procedure's icon, you will be presented with a menu of commands. This menu is called the procedure's command menu (or context) menu; sometimes, we simply call it the right-click menu. The menu includes commands that can be issued to the procedure that is currently selected.

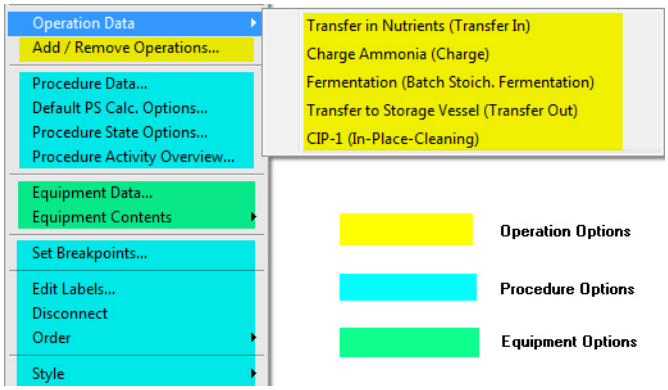


Figure 5.1: Command (context) menu for a unit procedure.

Please note that the contents of the menu do not depend on the unit procedure type (Chromatography, Filtration, etc.).

5.1b A Unit Procedure in a Batch Process

When modeling a batch process (also mentioned as a batch recipe) you may think of a batch unit procedure as simply a set of sequential operations; for example: 'Charge A', 'Charge B', 'Heat', 'Stir', 'React', 'Transfer Out'. A unit procedure may include any number of operations. Even though the operations are listed sequentially, they may be timed to occur concurrently. For example, you may specify to have operation 'Stir' execute continuously while 'Charge A', Charge B' and 'React' are set to execute concurrently (see 5.11d The Scheduling Group of Variables).

A unit procedure typically engages some kind of **main equipment resource** (Reactor, Fermentor, Diafilter, Nutche filter, etc.). In batch processing, two or more unit procedures can share the same main equipment resource. However, you must make sure that they are scheduled to execute in such a way that their equipment resource occupation times do not overlap. If this happens inadvertently, the program will generate an error message during simulation notifying the user that an equipment sharing violation has been detected.

The types of operations that can be included in a unit procedure depend on the type of equipment resource (Reactor, Diafilter etc.) hosting the procedure and the operating mode of the unit procedure (batch or continuous).

*Once a given procedure type is selected (from the list under the main menu **Unit Procedures**) then the equipment type assumed as a host is automatically selected. For example, if you select to include a gel filtration procedure, the equipment resource assumed as a host is always a GFL chromatography column. If there could be different hosts for the same procedure, then a separate entry in the **Unit Procedures** menu will be present. For example, there could be any one of several different host equipment for a batch vessel procedure: a stirred tank reactor, a fermentor, a seed fermentor, etc. For each supported equipment host a distinct entry exists under the **Unit Procedures ▸ Batch Vessel Procedure** menu option.*

5.1c A Unit Procedure in a Continuous Process

When modeling a continuous process (e.g., a typical wastewater treatment plant), you may think of a (continuous) unit procedure as simply a single unit operation: a CSTR or an aeration basin simply represents a container vessel that receives flow continuously, processes (reacts) continuously and outputs flow continuously. Since the (single) operation represented by the unit procedure is active ('on') all the time, a continuous unit procedure cannot share its equipment resource.

5.1d Common Features

Each unit procedure is represented on the flowsheet by an equipment-looking icon. There may be one or more input streams attached to the unit procedure as well as one or more output streams leaving the unit procedure. Every unit procedure is assigned a main equipment resource of the type that is required for that procedure type. However, as mentioned in A Unit Procedure in a Batch Process, in the case of batch processes, more than one unit procedures (of the same type) can be set to use the same equipment resource.

Even though you may be tempted to treat each icon shown on a flowsheet as representing equipment, you shouldn't unless the process (and all unit procedures) are in continuous mode. In batch mode, always think of each icon as representing a set of actions executed in an equipment resource of the type indicative by the appearance of the icon. There may be one, several or no actual equipment behind a processing step represented by an icon on the flowsheet.

Under a unit procedure icon you can see two labels displaying three name tags. The first label (**name label**) displays a string that is made up from three parts:

(a) the name of the unit procedure,

(b) a name-separator (defaults to a '/' character) and

(c) the name of the hosting equipment resource.

The second label (**description label**) is shown as a separate line and displays a short description of the unit procedure. Sometimes there will be some other small indicator bitmaps

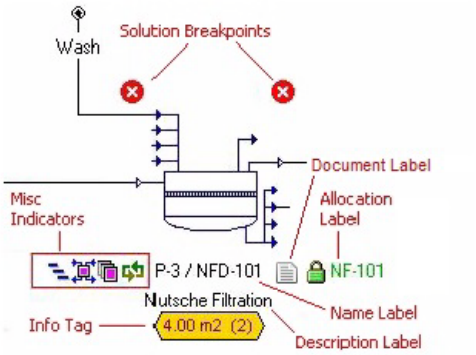


Figure 5.2: Labels and indicator bitmaps shown around a unit procedure icon.

appearing across the top or the across the bottom of the procedure's icon. All bitmap indicators that may appear across the top of the icon are related to the presence of breakpoints (see 8.15 Simulation Breakpoints). Occasionally, when the simulation is paused by the presence of a

breakpoint, there may be more bitmap indicators showing under the procedure icon. Those bitmaps indicate the solution state of the procedure (for more details, see 8.15 Simulation Breakpoints). Finally, some other small bitmap indicators may appear at the bottom left or bottom right of a procedure's icon. These bitmaps may remind the user of certain special circumstances surrounding the function of the procedure (e.g. multiple cycles or multiple equipment units, etc.).

Please note that the general appearance of a procedure's icon (including its labels and presence or absence of bitmap indicators around the icon) is determined by its drawing style. For more details on the meaning of each bitmap indicator and how to turn them on or off, see 5.7 Unit Procedure Icon Style.

5.2 UNIT PROCEDURE OPERATING MODE

A unit procedure's operating mode can be set as:

- Batch / Semi-Continuous, or
- Continuous

Some procedure types are inherently batch (e.g. chromatography). For those procedures the continuous mode options is disabled. On the other hand, any procedure, even those that are inherently continuous (e.g. pumping or a continuous reaction in a CSTR) can be set to semi-continuous operating mode, if needed. In this mode, the procedure is 'on' for some time (executing in its natural continuous mode), then it may be shut down for a period of time (i.e., it is 'off') as it may not be needed in the context of a batch process. A more intriguing situation appears when a batch procedure is set to operate in a continuous process. For example, suppose there is a batch vessel procedure in a reactor, executing a set of operations like: 'Charge', 'Heat', 'React' and 'Transfer out'. SuperPro Designer bridges the gap between the continuously flowing material around the procedure to the 'mini-batch' executing inside this procedure by assuming that the continuous material entering and leaving the procedure will be held up in some collecting tank(s) - not shown on the flowsheet. The time used to collect this material (**holdup time**) may be set by the user or it may be dictated by the operating requirements of the batch procedure (see 5.2a Holdup Time). On the other hand when a continuous procedure is set to operate in a batch process, then its throughput will be based on a batch amount processed per recipe cycle time. You can set the operating mode of a unit procedure through its Procedure Data Dialog.

A continuous procedure is, by default, 'on' all the time. However, in a batch flowsheet, the start time of a continuous procedure can optionally by set by scheduling its single operation with respect to other procedures in the recipe. If this is not done, then the continuous procedure will be assumed to start at time zero of the simulation horizon.

5.2a Holdup Time

When a batch unit procedure, such as chromatography, is set to operate in a continuous surrounding, SuperPro Designer needs to infer the amount of material that gets processed per cycle. The implicit assumption is that in order for this unit procedure to function cyclically in an otherwise continuous environment, there must be a tank that accumulates material for a

certain time (at least while the procedure is in progress) and then feeds the next cycle of the unit procedure. This time we call **holdup time**. Obviously, this time must be at least as long as the duration of the unit procedure (but it could be longer). For unit procedures whose cycle duration is set directly by the user (in other words, all contained operations have process times, setup times and turnaround times directly set by the user) the holdup time is assumed to be equal to the duration of the entire unit procedure. In that case, the user does not need to supply the procedure's holdup time (its field will not be editable in the procedure's operating mode dialog). However, if the duration of at least one operation of the unit procedure is calculated by the system, then the user must set the holdup time (the field is editable). Care must be taken to set the holdup time to a reasonable value: if the value set is too small, then there will not be enough time for the contained operations to execute; if the value is set too high, then the accumulated material that needs to be processed per cycle of the unit procedure becomes too large and if some of the contained operations' process times depend on the amount of material processed, then their operating times become too large, leading to a process cycle time that may be too large (or at least larger than the set holdup time). It is very easy to de-stabilize the interdependency between equipment capacity and holdup time if the process time calculation of at least one of the operations in the procedure's queue, depends linearly on the amount processed: Higher holdup times lead to larger capacity demands which in turn lead to higher process times (and procedure cycle times) that raise the lower limit on holdup times. An effective way to circumvent this self-feeding cycle is described below:

A challenging case involving the holdup time appears when all contained operations have their times set by the user. As mentioned previously, in that case, the holdup time is calculated by the program as the time between the start of the first operation and the end of the last operation. If that time happens to be very large and independent of the amount processed per cycle (e.g. it could be due to large reaction/fermentation time) then the sizing demand on the hosting equipment resource may be exceedingly large. To circumvent this predicament you can set the hosting equipment resource to operate in a staggered mode. In that case, the effective value used to estimate the amount of material processed per cycle would be the cycle time divided by N+1, where N is the extra sets of staggered equipment resource units, thereby reducing the capacity demands. For more details on the staggered mode of operation see 6.1c Staggered Mode.

5.2b Procedure Cycle and Cycle Duration

A unit procedure is assumed to capture the execution of a sequence of operations. A completed sequence of operations from the beginning of the first to the end of the last operation (as defined in the procedure's operation sequence list) is called a unit procedure **cycle**, and the time elapsed from the beginning of the first operation to the end of the last operation in the sequence is called the unit procedure's **cycle duration**.

*The cycle duration is not necessarily the sum of the execution times (durations) of the operations in the procedure's queue since there may be some operations that do not start as soon as the previous operation in the sequence ended (in other words, there may be some **idle time** between back-to-back operations in the sequence). Also, it may be that two (or more) operations may have durations that overlap each other (e.g. two consecutive charge operations and a reaction operation may span a time during which an agitation operation is supposed to be carried out. Such time may be necessary to simulate a simultaneous stirring while charging and having the contents of the vessel react.*

When an operation in the sequence of a procedure is processing material as part of a single batch, sometimes the demand for equipment resource capacity is such that it necessitates the

use of multiple units (in other words, there's not enough capacity to process the material through that step in one run). Very often, due to economic considerations (e.g. if the associated equipment is very expensive) or perhaps due to under-utilization of a given equipment resource, instead of engaging multiple equipment units in parallel, the material to be processed per single batch is split into a number of 'mini-batches' and each mini-batch is processed separately through that equipment. For example, consider the case where a large amount of material needs to be passed through a chromatography column. If the column's total cycle duration (including equilibration, loading, wash and regeneration) is relatively small compared to the time between batches (**process cycle time**), then instead of demanding the use of multiple columns (say 5), it may be preferable to divide the material into 5 equal amounts. These 5 mini-batches of material are processed by the column one-by-one, and the product streams and wastes are later merged back into a single product stream and a single waste stream. SuperPro Designer makes it very easy to accommodate such processing requirements, without having to show the actual split of the material into 5 cuts and represent each chromatography step separately (this would require 5 distinct icons with products that later merge together). The key is to set the **number of cycles** parameter of that procedure to a number larger than one (the default value); in our case 5. When this is done, SuperPro Designer will assume that the sequence of operations contained in the unit procedure (equilibration, load, wash and regeneration) will repeat itself in an identical manner. Each such sequential execution of operations (**cycle**) is assumed (by default) to tightly follow the cycle before it (i.e. there are no time gaps between the successive execution of consecutive cycles). Therefore, the **cycle time** (i.e. the time interval between consecutive cycle starts) is equal to the **cycle duration**. If a procedure has been set to have multiple cycles, then there is an option for the user to set the cycle time to any desired value. If the user-defined cycle time is smaller than the cycle duration, then multiple units (operating in staggered mode) will be needed; these extra pieces of equipment will be drawn from the staggered equipment pool (see Equipment Data Dialog: Equipment tab). If there are no staggered equipment specified on the Equipment Data Dialog, then processing of overlapping cycles is infeasible and SuperPro Designer will issue a scheduling error..

Note that you cannot use the start or end time of an operation in any intermediate cycle as the start time reference for the scheduling of other operations. When the start time of an operation (in a multi-cycled procedure) is selected as a reference point, then the start time of the operation as part of the first sequence of operations (cycle) is used. When the end time of an operation (in a multi-cycled procedure) is used as a reference time point, then the finish time of that operation, as part of the last cycle, is used. If you need to schedule or reference start or end times of operations during any of the cycles of a procedure, then it is recommended that you represent each cycle as a separate unit procedure (hosted by the same equipment resource). If you need to have some action(s) happen before the first cycle only or after the last cycle only, then that is another reason that you must represent each cycle as a separate unit procedure (hosted by the same equipment resource).

The periodic repetition of a unit procedure across batches is assumed, by default, to follow the pace dictated by the **recipe cycle time**. Optionally, however, it is possible to declare that a batch procedure has its own pace for repeating its cycle(s), i.e., **independent cycling**. In such a case, the procedure is executed with a periodicity that is different from the recipe's cycle time. This independent period (or **procedure cycle time**) can be set explicitly by the user as soon as he/she declares the procedure as 'cycling independently of main recipe' on the Procedure Data Dialog: Scheduling Tab. Alternatively, the user may specify how many cycles of this procedure are to be completed per cycle of the main recipe (**equivalent procedure cycles**). From this

number (which can be non-integer: greater than 1 for procedures that repeat themselves with a pace faster than the main batch, or smaller than 1 for procedures that repeat themselves with a pace slower than the main batch), the program will infer the appropriate procedure cycle time. The amount of material processed per each repetition of a procedure with independent cycling is calculated by dividing the material per batch with the number of equivalent cycles. The start time of the first execution of a procedure with independent cycling is implicitly inferred by the program from examining the start time of the first operation in the procedure's sequence. Such timing can be tied to any event of the main recipe: the start of the main recipe, or the start or end time of any other operation that is part of the main recipe. Please note that the inverse is not allowed: in other words, the scheduling of any operation in the main recipe cannot be tied to the start or end time of an operation that is part of an independently cycling procedure.

The number of cycles, declaration of a unit procedure as **independently cycling**, and the cycle time specification or the number of equivalent procedure cycles can all be set or viewed from the Procedure Data Dialog: Scheduling Tab...

*For an example of how to use a procedure which **cycles independently** of the main recipe, please refer to the Lysine example which ships with SuperPro Designer. This file contains several procedures which cycle independently. Additional information related to these types of procedures is available within the MS Word document associated with the Lysine example. The MS Word document in the Lysine folder also contains additional scheduling tips related to the use of staggered mode, use of batch and continuous procedures within the same flowsheet, schedulable start specifications for continuous procedures, etc.*

5.3 OPERATION SEQUENCE

Unit procedures contain a sequence of one or more operations. Most unit procedures contain already an operation by the time they are first created. For instance, when you insert a microfiltration (batch) unit procedure, it already contains a 'Batch Concentration' operation. You can, of course, add more operations later. Some unit procedures contain no operations when they are first created. For example, all the Batch Vessel Procedures (in a Reactor, in a Fermentor, in a Seed Fermentor, etc.) start out without any operation in their sequence and therefore they simulate no action. They are considered 'general purpose' unit procedures and as such they do not contain (by creation) any pre-determined operations. You must visit their 'Add/Remove Operations' dialog (aka The Operation Sequence Dialog) and add operations to them. Operations can be added/removed/re-ordered in a unit procedure by right-clicking on the unit procedure's icon and then selecting the **Add / Remove Operations** option. Remember that a unit procedure has a dual behavior depending upon its operating mode. If it is a continuously operated procedure, then one and only one operation can be carried out by this unit procedure and the **Add/Remove Operation** menu option will not be available in the context menu of this unit procedure.

As a shortcut, you can access The Operation Sequence Dialog of a unit procedure in batch mode by double-clicking on its icon. Double clicking on a procedure that is set to operate in continuous mode will bring up the i/o dialog of the (only) operation in it.

Note that you can add as many operations as you wish in the operation list of a batch unit procedure. However, the types of operations available depend on the specific type of unit procedure you are editing. For example, for a Microfiltration (Batch) unit procedure the available options for operations are:

1. CIP (Clean-in-Place)
2. Concentrate
3. Flush
4. Hold
5. SIP (Steam-in-Place)

In a Gel Filtration procedure on the other hand the list of available operations are:

1. CIP (Clean-in-Place)
2. Elute
3. Equilibrate
4. Hold
5. Load
6. Regenerate
7. SIP (Steam-in-Place)
8. Wash

From The Operation Sequence Dialog (aka 'Add/Remove Operations' dialog) you can also rename an operation currently in the list and even reorder the list.

It is very important to understand that for material and energy (M&E) balances, when the time comes to simulate the process step represented by a unit procedure, SuperPro Designer's simulation engine executes the actions that each operation represents one-after-another (always) and in the order that they appear in the unit procedure's list. For example, if you insert first a 'Charge-A' then a 'Charge-B' and then a 'Heat' operation, this is exactly what will be simulated. For timing purposes, you can set the durations and start times of all these operations to coincide (if that is what actually happens). So, you can set the start time of the 'Charge-A' to coincide with the start time of 'Charge-B' as well as the start time of 'Heat' and you can set the durations of 'Charge-B' and 'Heat' to be the same as the duration of 'Charge-A'. For more information on how to set the timing of operations, see 5.11d The Scheduling Group of Variables. Note that it is possible that the final outcome of the mass and energy balance calculations to be different depending on the operation order.

As you add new operations to the procedure sequence, their scheduling settings are set automatically by the program in an intelligent manner: The first operation is assumed that its start time will be determined using a time shift (set by default to 0.0) with respect to the beginning of the batch. In other words, the program assumes that the first operation of a unit procedure (and hence the procedure itself) will start at the beginning of the batch. Every subsequent operation is scheduled to start as soon as the previous operation in the queue is ended; in other words, it uses as reference time the end of the previous operation and as time

shift 0.0. All of these settings of course, can be changed. Simply visit the Operations Dialog: Scheduling Tab of each operation in the list and modify accordingly.

Quick View of the Activities under a Unit Procedure

If you move the mouse over a unit procedure's icon and **shift+click** right over the icon, you will be presented with a popup window that shows (in brief) a line-by-line description of all the activities that are currently set to execute in that procedure. Figure 5.3 shows what is being presented after shift+clicking on the fermentation procedure of the b-gal example (supplied with the software).

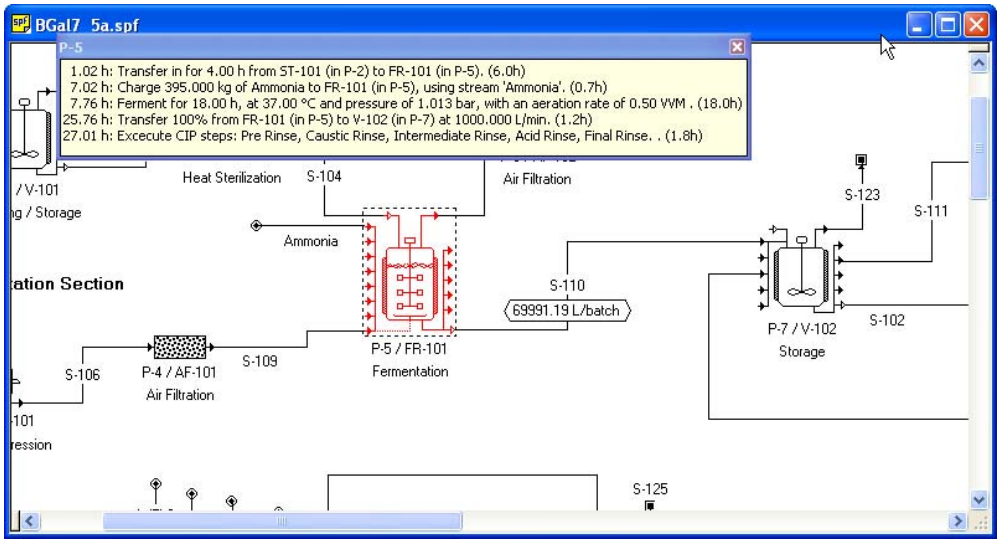

BGal7_5a.spf
P-5
1.02 h: Transfer in for 4.00 h from ST-101 (in P-2) to FR-101 (in P-5). (6.0h)
7.02 h: Charge 395.000 kg of Ammonia to FR-101 (in P-5), using stream 'Ammonia'. (0.7h)
7.76 h: Ferment for 18.00 h, at 37.00 °C and pressure of 1.013 bar, with an aeration rate of 0.50 VVM . (18.0h)
25.76 h: Transfer 100% from FR-101 (in P-5) to V-102 (in P-7) at 1000.000 L/min. (1.2h)
27.01 h: Excecute CIP steps: Pre Rinse, Caustic Rinse, Intermediate Rinse, Acid Rinse, Final Rinse. . (1.8h)
Heat Sterilization
S-104
Air Filtration
S-123
S-111
Ammonia
S-110
69991.19 L/batch
P-7 / V-102
Storage
S-102
P-5 / FR-101
Fermentation
S-109
P-4 / AF-101
Air Filtration
S-106
S-125

Figure 5.3: Quick-view of a unit procedure's activities using the shift+click mouse action.

The information presented for each operation has three parts:

1. The first part indicates the absolute start time of the operation. Note that this time may either be set by the user directly or it could be calculated indirectly (based on a start time reference operation and a start time shift as set on the Operations Dialog: Scheduling Tab).
2. The second part is a short description of the operation constructed based on the user's specifications (e.g. amount transferred or charged, temperature settings, etc.) and as shown in the Operations Dialog: Description Tab. The description can also be customized, if necessary, to suit your preferences.
3. Finally, the last part (shown in parenthesis) indicates the duration of the operation.

The fly-over window can be moved anywhere on the screen (by clicking-and-dragging its title bar that displays the name of the procedure); it can be closed down by either clicking on the top-right **Cancel** button ( ) or simply clicking away from it.

The units of measure chosen to display the times and operating parameters in the description of each operation are the same as what is used to display the same information on the operation's i/o simulation dialog. The defaults (for all operations) are set at the process level (see 8.4 Units of Measure (Physical Units Options) but they can be customized for a given operation from its i/o simulation dialog .

Quick View of a Stream's Utilization by a Unit Procedure

Another related popup window appears when you **shift+click** on a stream hooked up to a procedure. This time the popup that appears presents information that explains how the stream is being utilized by the unit procedure.

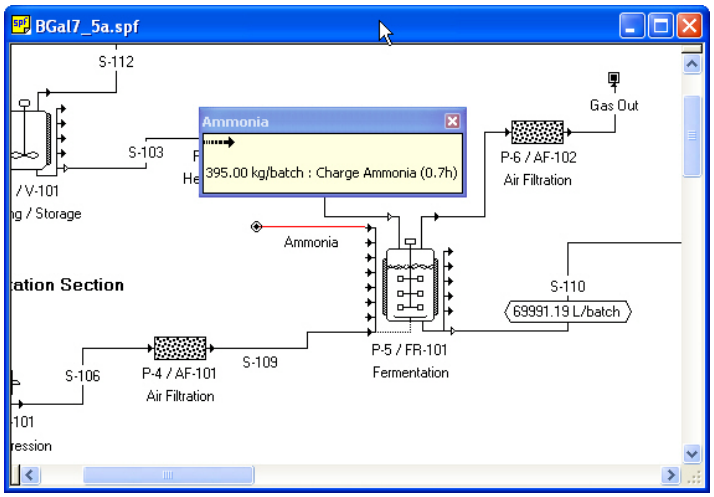


Figure 5.4: Quick-view of a stream's utilization using the shift+click mouse action.

For example, the popup above conveys the information that stream "Ammonia" carries 395 kg/batch and it is used by the operation named "Charge Ammonia" whose duration is 3.7h. Such information can be very useful when a unit procedure has several input and/or output ports and it includes a long list of operations in its operation sequence.

5.4 UNIT PROCEDURE ICON

Each unit procedure is represented on the flowsheet by a unique icon. The actual image used depends upon the type of equipment resource that this procedure utilizes (e.g. a Vessel, a Chromatography Column, etc). Unlike what the image suggests, please note that when SuperPro Designer is used to model batch processes, each icon on the screen represents a unit procedure (aka a process step) and not a piece of equipment. Multiple unit procedures may utilize the same equipment resource (at different times) and therefore, they may be represented multiple times on the process flowsheet (even though they employ the same equipment resource). For continuous processes that are carried out by continuous procedures, interpreting an icon as a piece of equipment is not quite inaccurate. One only needs to remember that it is possible to have a single continuous step (unit procedure), represented on the flowsheet with a single icon, be actually carried out by multiple pieces of equipment (operating in parallel and/or staggered mode as specified through the Equipment Data Dialog: Equipment tab). It is very important to remember that a unit procedure icon presents the visual communication element to view and edit data that are related to three different entities:

1. The Unit Procedure itself,
2. The Equipment Resource hosting the unit procedure, and

3. Any of the Operations included in the unit procedure's sequence.

The command menu of the icon (that is the menu that appears when you right-click over an icon) presents options that are related to all of the above:

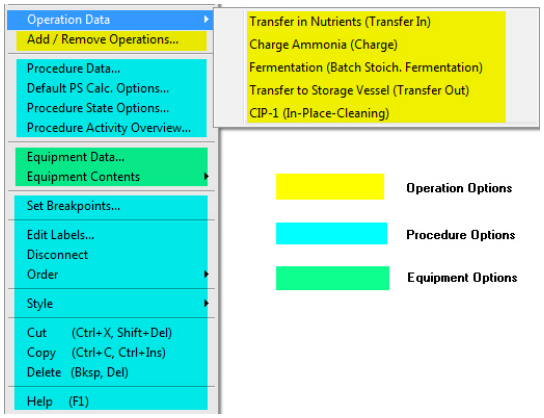


Figure 5.5: The unit procedure's command menu (aka context menu or right-click menu).

5.5 UNIT PROCEDURE PORTS

Material flows in and out of unit procedures via streams, see Streams. Streams engage to specific locations on a unit procedure called **ports**. A port is simply a connection point that can be used by an incoming or an outgoing stream. **Input ports** are those used as ending points of streams with flow into the unit procedure and **output ports** are touch points for streams that represent material leaving the unit procedure. Since there are two types of material flows (bulk and discrete) (see 4.1 Types of Streams) there are also two types of ports: **bulk flow ports** and **discrete flow ports**. Only bulk streams can use bulk flow ports and only discrete streams can use discrete flow ports. Note that input/output bulk ports are drawn slightly differently from input/output discrete ports

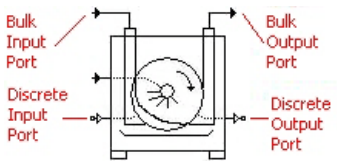


Figure 5.6: Bulk and discrete, input and output ports around a unit procedure icon.

The location of each port can be easily recognized since the mouse pointer changes as soon as the mouse is over a port:

- 'Bulk Flow Port' pointer (input or output):

- 'Discrete Flow Port' pointer (input or output):

Output ports serve as starting points for intermediate and output streams and input ports serve as ending points of intermediate and input streams. Having the mouse pointer change when the system detects that it is over a port, greatly facilitates the drawing of a stream since it makes it very easy to locate the start point (some output port) or end point (some input port) of a stream (if the stream is attached to a unit procedure). Please note that an input port that may already have a stream attached is considered 'busy' by the system and therefore it is unavailable as an ending points for an input stream. Similarly, an output port with a stream already hooked on to it, is also considered 'busy' and therefore, it is not available as a starting point for an output or an intermediate stream.

Some procedure types are hosted by an equipment resource that allows for both a bulk and a discrete port. For instance, consider the Filling procedure shown in Figure 5.7.

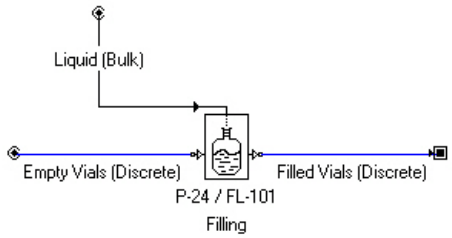


Figure 5.7: The 'Filling' procedure features a bulk input and a discrete input port and a discrete output port.

One feed (input) line provides the empty vials (bottles) and it is connected to the discrete input port. The other feed (input) port allows for the liquid material (in bulk) to be brought in and used to fill up the vials. Of course, the single output line (stream) of the procedure is a discrete line of filled vials, and therefore it requires a discrete output port.

5.5a Default Input Ports & Auto-Initialization

Out of all input ports, one of them is special and considered as the **default input port**. The default input port has the following special property: it allows the material of the stream attached to it to be automatically forwarded (pushed) into the unit procedure's equipment (i.e., without the user having to define a special 'Transfer in' or 'Charge' operation). This function is called the **auto-initialization** of a unit procedure. The auto-initialization of a unit procedure is only activated if the unit procedure is set to operate in batch mode and it doesn't have any operations in its operation sequence that themselves transfer in any material. This behavior presents a very convenient way to transfer material into a unit procedure without having to worry about their timing (scheduling).

The auto-initialization of a batch unit procedure is active only if there are no operations in the operation sequence that transfer material into the unit procedure (e.g. a transfer-in, charge, pull-in, etc.) and of course, if there is a stream attached to the default input port. In other words, you must either completely disregard the timing (scheduling) of all material entering a procedure or schedule all of it.

Notice how SuperPro Designer displays the default input port with a hollow arrow whereas all other ports are displayed with a solid arrow:

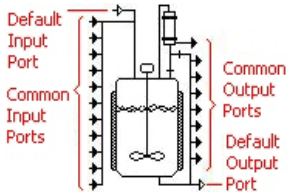


Figure 5.8: The default input and default output ports are drawn differently (hollow arrow).

5.5b Default Output Port & Auto-Removal

The **default output port** is a similar concept applied to the output of material from a unit procedure. The default output port is a designated port that automatically transfers out of the equipment contents any material remaining after the conclusion of the last operation to the attached stream (assuming that the hosting equipment has the ability to hold material.) This behavior of a unit procedure is called the **auto-removal**. Just like the auto-initialization the auto-removal is a convenient way to remove material without having to worry about the timing (scheduling) of the removal operation.

The auto-removal of a batch unit procedure is active only if there are no operations in the unit procedure's queue that remove material to a stream and of course, only if there is a stream attached to the default output port. In other words, you must either completely disregard the timing (scheduling) of all material leaving a procedure or schedule all of it.

The notion of the default input and/or output port also exists on icons representing procedures hosted by equipment that are meant to be functioning in a continuous (or semi-batch) mode: for example, a multi-effect evaporator, a thin-film evaporator, an absorber or a stripper. In such continuously operated equipment that may have more than one inputs or outputs, the default input (or output) port is used to indicate the 'main' feed (or outlet) of the procedure. In other words, the main input/output indicate where the process stream is expected to be connected. In continuous procedures the notion of auto-initialization or auto-removal does not apply.

5.6 UNIT PROCEDURE LABELS

Each unit procedure icon is accompanied by three basic labels:

1. The Name Label
2. The Description Label
3. The Allocation Label

The allocation label appears rarely and it is only relevant if the equipment resource hosting the the unit procedure has been allocated to either a site equipment or an equipment vendor specification (see 6.1i Equipment Allocation).

The description label, simply displays a string that is supposed to convey to a viewer what is being accomplished by the unit procedure (e.g. Bacterial Fermentation).

The name label by default reports the name of the unit procedure and the name of the equipment resource that is used to carry out the procedure. The two names (unit procedure name and equipment resource name) are separated by a '/' (separation delimiter). The separation delimiter is part of a procedure's style and can be changed by the user to any string through the Unit Procedure Icon Style Dialog: Name Label Tab. By default, SuperPro Designer makes up a name for new unit procedure by combining a prefix (originally set to be 'P-') and a number starting with 1. For example, the first unit procedure will be named 'P-1'. The next unit procedure will be called 'P-2', and so forth. The equipment tag names are made up in a similar way, except the prefix depends on the type of equipment being employed. For example, for vessels the prefix is 'V-' and for microfilters is 'MF-'. Following this rule, 'V-101' will be used as the first vessel's name and 'V-102' will be used for the second vessel, etc. Both the prefix ('P-'or 'V-' etc.) and the starting number can also be changed, see 8.20 Application Settings). All unit procedure names must be unique amongst unit procedures and all equipment resource tags must be unique amongst equipment resource tags. Both the name and the equipment tag name are user-editable (from the Edit Procedure Labels Dialog) and can be hidden (if desired). The settings for showing or hiding a procedure's or its equipment resource name are kept as part of the Unit Procedure Icon Style and can be edited from the Unit Procedure Icon Style Dialog: Icon Tab.

The fonts, colors, frames and other display attributes used by the system to display the labels of a unit procedure are also dictated by the Unit Procedure Icon Style. As soon as a unit procedure is created, it inherits a default style that is part of the process settings (see 8.3 Default Style for Process Elements). Both the default style for a unit procedure and the individual style of a given procedure can be modified. To modify the default style of all procedure icons, select **Edit ▸ Process Options ▸ Preferences ▸ Default Styles ▸ Procedure Icons** from the main menu or **Preferences ▸ Default Styles ▸ Procedure Icons** from the flowsheet's context menu. You can change the style of a particular unit procedure through the Unit Procedure Icon Style Dialog. To display this dialog, right-click on the procedure icon and select **Style ▸ Edit**.

5.7 UNIT PROCEDURE ICON STYLE

The style of a unit procedure icon is a collection of attributes that determine the visual appearance of the icon, its labels and any surrounding indicators. Icons of unit procedures are monochrome. They are drawn using a default color that is part of the default style for a procedure. The labels are drawn using a font and text color that is also part of the default style of a procedure. The default unit procedure style is a property of the document itself. To modify the default style of icons select **Preferences ▸ Default Styles ▸ Procedure Icons** from the flowsheet's command menu. From that dialog you can edit the style and therefore the appearance of all current (and future) procedure icons. You also customize the appearance of a specific icon by visiting the Unit Procedure Icon Style Dialog for the corresponding icon. To view the icon's style dialog select the **Style ▸ Edit** option from the icon's command menu.

The following table shows all the attributes that make up the style of a procedure's icon:

Icon	- Color. - Show/hide name label, description label, allocation label, info tag. - Show/hide Indicators for multiple cycles, multiple units, shared equipment resource, staggered equipment resources, independent cycling, comments.
Name Label	- Content (procedure name and/or equipment name). - Text: font, color, background color. - Frame: shape, line thickness, line color, fill-in color.
Description Label	- Text font, color, background color. - Frame shape, line thickness, line color, fill-in color.
Allocation Label	- Text font, color. - Frame shape, line thickness, line color, fill-in color.
Info Tag	- Content (choose variables to be displayed). - Text font, color. - Frame shape, line thickness, line color, fill-in color. - Location: top of the icon, over the icon, below the icon.

Once you have customized the appearance of a given icon, this icon will be protected from any future changes in the default procedure icon style. If you decide to force the icon to forgo its custom style and follow the default icon attributes, then select the **Style ▸ Use Default** option from the icon's command (right-click) menu. If you have customized the appearance of an icon and now you wish to propagate the same changes to one (or more) other icons, use the following procedure:

▶ **To copy a pre-existing style from one icon to another (or others)...**

1. Select the icon that features the style that you wish to copy.
2. From the command menu of the selected icon, chose **Style ▸ Pickup**; alternatively you can click the **Pickup Style** button () on the drawing palette.
3. Select the other icons that you wish to apply the selected style.
4. Right-click on any of the selected icons and from the command menu select **Style ▸ Apply**; alternatively you can click the **Apply Style** button () on the drawing palette.

5.8 UNIT PROCEDURE TYPES

A detailed list of all unit procedure types available to be included in a process simulation is only available in the PDF version of the manual or as part of the on line help documents. The actual list of available options depends on which member of the Pro-Designer family of software you own (EnviroPro or SuperPro). If you want to view the available operations for an existing unit procedure, you can do one of the following:

▶ **To view documentation about an existing unit procedure (e.g. type of equipment host, available operations, input/output port description)...**

1. Select the unit procedure's icons.
2. From the command menu of the procedure, select **Help**; alternatively, you can simply hit the **F1** key as a shortcut. The online help documentation system will present directly a topic relevant to this procedure's type. On that topic you can find a detailed listing of all the operation types available for the chosen procedure, the equipment resource type that is assigned to host the procedure as well information on any special role (if any) some of the input or output ports may play.

5.9 WHAT IS A UNIT OPERATION?

A **unit operation** (aka, an operation) represents the simplest physico chemical transformation step that can be modeled by SuperPro Designer. It can represent a simple activity, such as 'Charge' or a 'Mix', or a more complicated activity, such as 'Distill' or 'React'. Operations are strung together to form a unit procedure and unit procedures are put together to make up a process (or a recipe).

Sometimes a unit procedure may simply include only one operation. This is actually the norm in continuous processes. In that case, a unit procedure is equivalent to a unit operation. In batch processing however, most unit procedures include more than one operations. In order to add or remove an operation from a unit procedure, you must use The Operation Sequence Dialog that appears when selecting **Add/Remove Operation** from the procedure's command menu. Remember that this dialog is only available if the unit procedure is in batch (or semi-continuous) mode. Not all operation types supported by SuperPro Designer are available in a given unit procedure. The actual list available depends on the type of unit procedure and the type of equipment resource used to host the procedure. The operations available for the procedure are listed on the left pane of The Operation Sequence Dialog. The right pane shows the actual operations that have already been assigned to execute currently in the procedure.

A typical unit operation has many attributes; some are very specific to the nature of the operation and some are common to all operations. For example, a 'Heat' operation has as one of its attributes the temperature target for the heating or the heating rate; these are attributes akin to this operation type alone. A 'Heat' operation also has attributes related to its scheduling. For example, it has a specification that dictates when the user expects the operation to start. Also, there may be some labor resources tied up when the operation is being carried out. These last two sets of attributes (and a few others) are common to all operations. All the attributes of an operation can be viewed and edited (if allowed) by its input/output (i/o) simulation dialog. Since the operations themselves do not have a direct iconic representation on the flowsheet, in order to bring up the i/o simulation dialog of an operation in a unit procedure, right-click on the procedure's icon and then select **Operation Data** (if only one operation is in the operation sequence). If several operations are included in the operation sequence, you must select the name of the operation that you want to view from the submenu under the **Operation Data** entry.

5.10 TREE-VIEW OF A PROCESS

You can choose to view a process (and all its procedures and operations) in a tree-like representation if you choose **View ▸ Utilization Breakdown ▸ Procedures** from the main menu of the application. The interface that appears will show in tree-like node-subnode representation the entire process. The user can customize which nodes are used as aggregates (possibly omitting the section and/or branch level). For more information on how to customize the contents of this interface, see View Procedure Utilization Breakdown.

5.11 THE INPUT/OUTPUT (I/O) SIMULATION DIALOG

The i/o simulation dialog of an operation is made up from several tabs. Each tab presents a group of variables. Some variables are required to be set by the user (inputs) and others are

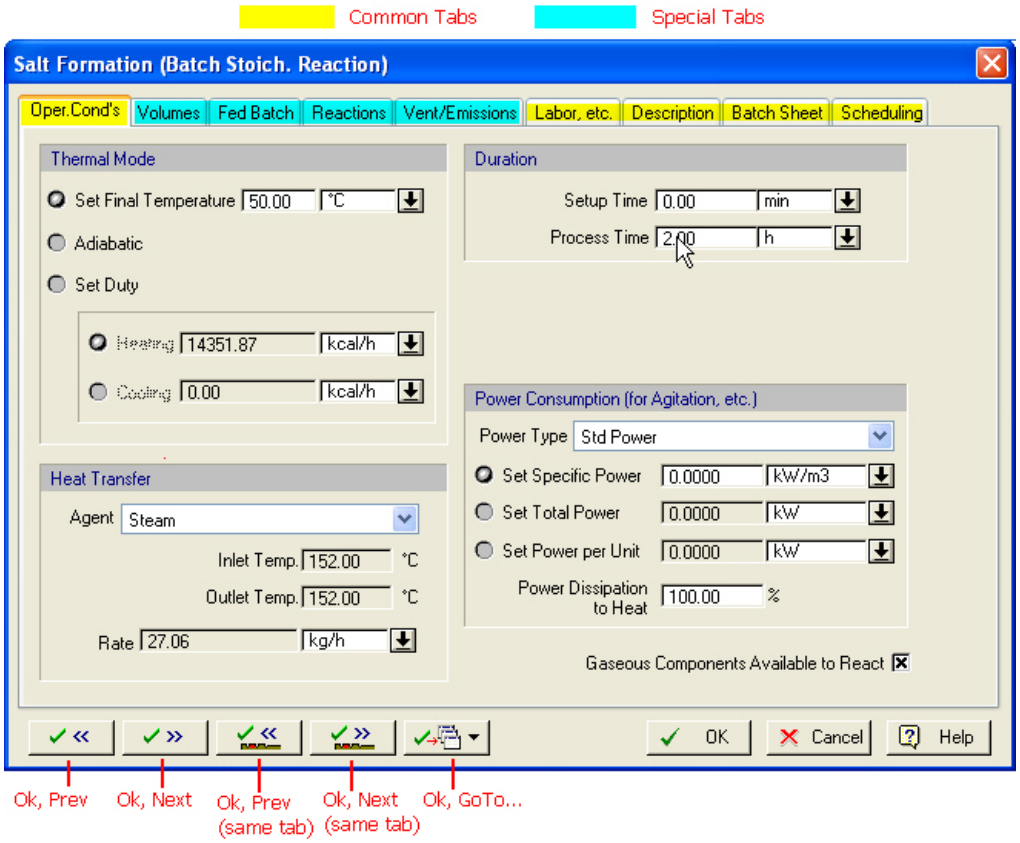


Figure 5.9: A typical input/output (i/o) simulation dialog for an operation.

calculated by the simulation engine (outputs). Sometimes a variable may be considered an input or an output depending on other operation-related or procedure-related settings (e.g. operating mode), or even equipment-related settings (e.g. sizing options). Most input variables come preset to some reasonable default values. A typical i/o simulation dialog is shown below (for the stoichiometric reaction operation)

As a shortcut to visiting another operation's i/o simulation dialog in the same unit procedure queue, this dialog offers (besides the regular **OK**, **Cancel**, **Help** buttons) another set of buttons that allow you to accept the changes in this dialog and automatically open the i/o simulation dialog of another operation (next or previous in the sequence order). The first two buttons open the next (or previous) operation dialog and show the first tab (typically the 'Oper.Cond's' tab) whereas the next two buttons open the next (or previous) operation's i/o simulation dialog at the same tab as the one being viewed currently (if it exists). Finally, the fifth button allows you to jump to another operation's dialog (not necessarily the next or previous in the sequence order). Note that moving your cursor over the buttons of the dialog will present a tooltip reminder of their functionality.

Even though the 'Oper. Cond's' tab is common to all operations, the contents of the tab (i.e. the variables that belong in this group) can vary significantly from operation to operation. The other four common tabs ('Labor etc'., 'Description', 'Batch Sheet' and 'Scheduling') when they appear they are exactly the same in all operations.

If you need to get some information related to the meaning or legal range of values for any of the parameters appearing on any of the dialog's tabs, just click on **Help** (or hit **F1** on your keyboard) and you will be presented with a topic that provides you with information related to the specific tab that you are viewing. Also, from the same help topic, you will find links that will lead to a detailed description of the modeling equations behind the specific operation.

5.11a The Labor Etc. Group of Variables

This group of variables focuses on covering the following three issues (common to all operations):

1. Labor Demand: There can be several types of labor that can be associated with the carrying out of an operation: plain operator type, supervisory labor, quality-control labor, etc. SuperPro will track the requirements of each labor type provided the user specifies for each operation what type of labor(s) is needed and at what rate (labor-hours per operation-hour or per cycle). If the type of labor that you wish to associate with an operation is not available already you can introduce new types (see 15.9b Adding or Deleting a Labor Type).
2. Auxiliary Utilities (heating, cooling or power) demand: Oftentimes, it may be required to dedicate extra amounts of utilities in the form of heating or cooling or power for reasons that are unaccounted by the simulation model of the operation. For each utility category you can specify the type and rate of consumption and then the calculated rates (and amounts) will be tacked on to the rates calculated by the model (if any). If the type of utility you need to assign is not available, you can introduce your own (see 15.7b Adding or Deleting a Heat Transfer Agent and 15.8b Adding or Deleting a Power Type).
3. Size (or Throughput) Utilization Factor: This number reflects the extent that the host equipment's capacity (or throughput) is being utilized by the current operation. For example, for a charge operation that carries in 1,000L in a 10,000L vessel, the utilization

factor is 10%. For operations that are hosted by equipment resources whose 'size' is measured by a throughput variable and not a capacity variable (e.g. a homogenizer) this ratio will be the effective throughput of the operation over the rated throughput of the host equipment. This measure is used in the throughput analysis calculations that estimate the throughput potential of an existing facility as well as pinpoint bottlenecks when attempting to expand the production level (see 11.1c Potential Maximum Throughput Size).

The property page displaying the above set of variables for each operation is always the Operations Dialog: Labor, etc Tab.

5.11b The Description Group Variables

This group of variables addresses two issues (common to all operations):

1. Verbal Description of the Operation: There are circumstances when SuperPro needs to verbally describe the events occurring in the process. For example, when we display the operation Gantt chart we can display right next to the activity bars a text description of what each bar represents (see 7.4 The Operations Gantt Chart (OGC)). Also, when shift+clicking over a unit procedure, a tooltip window appears that displays a brief overview of the activities included in that procedure (see 'Quick View of the Activities under a Unit Procedure' on page 5-9). The description settings of an operation dictate how SuperPro will put together a textual description that will use to represent this operation. Most operations have a short and a long textual description of themselves. Note that the description may include actual values of operating parameters (e.g. amounts charged, reaction conditions, etc.). The user may also choose to overwrite the pre-existing templates for the operation and provide his/her own description. Unfortunately that description will be supplied 'as-is' without employing any operating variables.
2. Comments: If you wish to associate any comments that may be reminders for you or another viewer of the process, this is the place to add them. For example, it may be of importance to note here sources for the values of settings chosen in the operation, or any other assumptions or simplifications made when approximating the real process event(s) with the operation chosen.

The property page displaying the above set of variables for each operation is always the Operations Dialog: Description Tab.

5.11c The Batch Sheet Group of Variables

This group of variables addresses how SuperPro Designer will describe this operation when generating the batch sheet for the process. The 'Batch Sheet' is a very long document that describes in great detail the actions involved in the execution of the recipe. Typically, each operation is described based on a template (or form) that is operation-type specific. SuperPro Designer instantiates each operation's type form for a given operation, fills in the template with the operational values required and adds the resulting description in a master document whose structure is also dictated by a master template. For more details on the Batch Sheet, see Batch Sheet Generation.

You may elect not to include a given operation in the batch sheet, or you may chose to utilize a textual description that is simply the description text of the operation. All the choices related to this group of variables are presented in the Operations Dialog: Batch Sheet Tab.

5.11d The Scheduling Group of Variables

This group of variables are always presented for viewing and/or editing on the Operations Dialog: Scheduling Tab and are used to capture the following attributes:

1. The start time of the operation
   SuperPro Designer calculates the start time of an operation using two settings:
   (a) A reference event and (b) a time shift (positive or negative) from that event.
   The reference event can be one of the following:
   (a) The beginning of the batch
   (b) The start time or end time of another operation in the same or another procedure.
2. The duration of the operation
   It is assumed that the entire duration of an operation is made up from three parts:
   (a) The setup time
   (b) The process time, and
   (c) The turnaround time
   Users may elect to specify each portion of the entire duration separately or lump them together in one or two values alone.

The process time of an operation can often be (optionally) calculated based on some performance variable of the operation: for example, a charge operation may compute its process time based on a user-specified charge rate. In some operations the process time is always calculated (e.g. Column Load in a chromatography column). When the process time can be calculated based on some other attribute of the operation, it is also displayed in the Oper. Cond's tab.

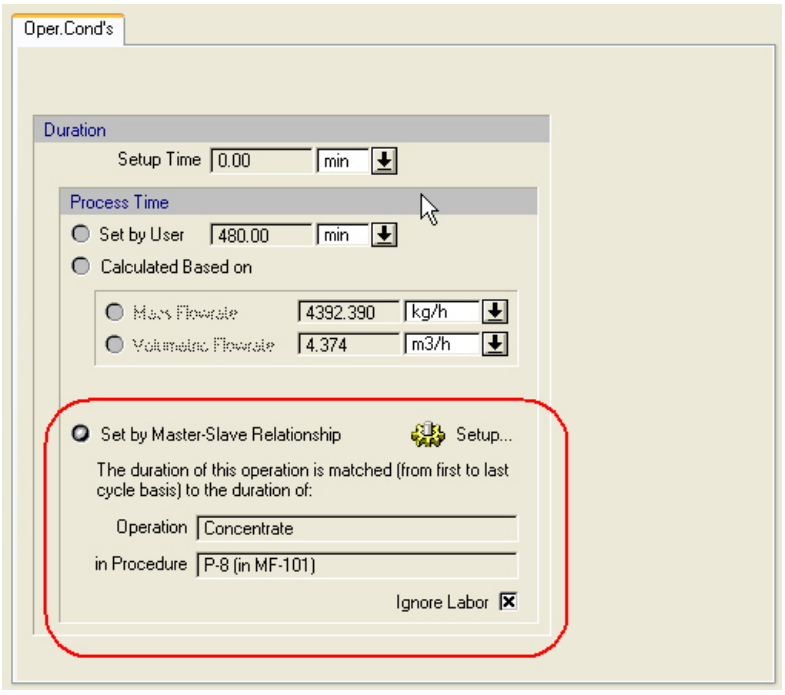


Figure 5.10: The process time can be dictated from a master-slave relationship.

As another alternative to calculate the duration of an operation, a user may elect to match the duration of one operation (master) to the duration of another (slave). This option is available to several operations and, when available, it is set from the Oper. Cond's tab of the operation (Figure 5.10). After selecting to set the process time by a master operation, clicking on the 'Setup' button will bring up the The Master-Slave Relationship Dialog that will allow the user to select the master operation.

5.12 PROCEDURE STATES

A unit procedure is assumed to be hosted by an equipment resource (the only exception from this rule are the transportation procedures that do not assume a host equipment). Unlike a continuous, steady-state operating process where all process steps require dedicated equipment resources 100% of the time, in a batch process, it is possible to utilize the same equipment resource (e.g. some storage unit) in distinct steps (procedures) of the process that happen at different time periods during the execution of a batch. Equipment sharing can be captured by SuperPro Designer, see Equipment Selection & Sharing. Most equipment are not pass-through (in nature) and therefore hold material during the sequence of execution of the several operations in a procedure. The equipment contents during the execution of a procedure are called (in SuperPro Designer' s terminology) **Procedure States** (or in some dialogs you may find the initials 'PS' for short). Then again, some equipment (e.g. a Dead-End Filter) do not have material holding capacity and therefore do not have any procedure states. Also, having or not procedure states may depend on just on the equipment itself, but how the procedure is being run (ie. in batch mode or in continuous mode). For instance, a Stirred Reactor Vessel, if utilized as part of a 'Batch Vessel Procedure' has procedure contents before and after every operation defined in its operation sequence. If, though, the same equipment is utilized as part of a CSTR continuous reaction, then the procedure does not feature any states.

5.12a Procedure State Physical State Calculation Options

Material in procedure states is considered to be in either vapor or liquid/solid state. For each procedure state, SuperPro Designer calculates the Physical State (PS) of each component by either a simplified component-specific set of criteria (i.e., the Shortcut PS Toolbox) or by an elaborate VLE Model (i.e., the Rigorous PS Toolbox). A detailed description of the physical state calculation options is given in 8.12 Physical State Calculation Options.

The PS of a procedure state is indicated by the vapor fractions of its components. The ***component vapor fraction*** *(i.e., the moles of the component in the vapor phase divided by the total moles of the component) must not be confused with the* ***molar fraction of the component in the vapor phase*** *(i.e., the moles of the component in the vapor phase, divided by the total moles of all components in the vapor phase).*

By default, every procedure state inherits the default PS calculation options of its associated unit procedure. It is possible to deviate from these default settings in one of the following ways:

1. *Modify the assigned PS Toolbox*. While the Shortcut PS Toolbox offers a quick way to determine the physical state of a procedure state, the Rigorous PS Toolbox calculates the distribution of components in the vapor and liquid/solid phase in a more realistic manner. As a rule of thumb, the Shortcut Toolbox should be used when the accuracy of physical

state calculations is not a primary concern or when no change of phase occurs in the process.

2. *Modify the options of the assigned toolbox.* For example, it may be necessary to change the Shortcut PS Toolbox V/L split criterion of a component (e.g., ammonia) from the default *Normal Boiling Point* to *Liquid/Solid Only* as it may be known that, at the conditions of the procedure state, all ammonia present in the mixture is dissolved in the liquid phase. On the other hand, given a procedure state that uses the Rigorous PS Toolbox (e.g. a mixture of hydrocarbons for which the binary interaction coefficients are readily available), an *EOS model* (e.g., the Peng-Robinson or the SRK) is best suited than the default *Raoult's law.*

CUSTOMIZING THE PS CALCULATION OPTIONS OF A PROCEDURE STATE

▶ How to select between the Shortcut or the Rigorous Toolbox...

1. While in select mode (i.e., the button is pressed on the main toolbar), right-click on the procedure icon and select **Procedure State Options**.
2. Each tab in this dialog corresponds to an operation in the procedure. The options in each tab apply to the calculation of the PS *after* the corresponding operation. Visit the respective tab of the procedure state whose PS calculation options you would like to change.
3. Check the Overwrite checkbox in the Physical State (PS) Calculation Options frame (see Figure 5.11).
4. Select between the Shortcut or Rigorous PS Toolbox option.

Figure 5.11: Selection between the Shortcut and the Rigorous Toolbox for the calculation of the stream's physical state.

For each procedure state (a.k.a. equipment contents), the selection between the Shortcut vs Rigorous PS Toolbox as well as the comprehensive PS Toolbox options are, by default, dictated by their associated procedure. This means that any change to the procedure's PS calculation options will be automatically propagated to all of its procedure states (as well as all output streams of that procedure). Checking the Overwrite option allows the procedure state to differentiate its behavior and adopt a different set of PS calculation options from its associated procedure. As a consequence, from that point onwards, any change to the PS calculation options of the procedure will not be propagated to that procedure state.

▶ How to customize the Shortcut Toolbox options for one or more procedure states in a procedure...

1. While in select mode, right-click on the procedure icon and select **Procedure State Options...**
2. Visit the respective tab of the procedure state whose PS calculation options you would like to change. Please remember that each tab represents the state of the procedure (a.k.a., equipment contents) right *after* the operation mentioned at the top of the tab.
3. Check the Overwrite checkbox in the Physical State (PS) Calculation Options frame.
4. Make sure the Shortcut Toolbox option is selected.

5. Check the **Custom?** checkbox for the specific component you wish to change the V/L split criterion (see Figure 5.12).
6. From the V/L Split Criterion drop-down list, select the criterion of choice (see 8.12a The Shortcut Physical State Calculation Toolbox for more details).

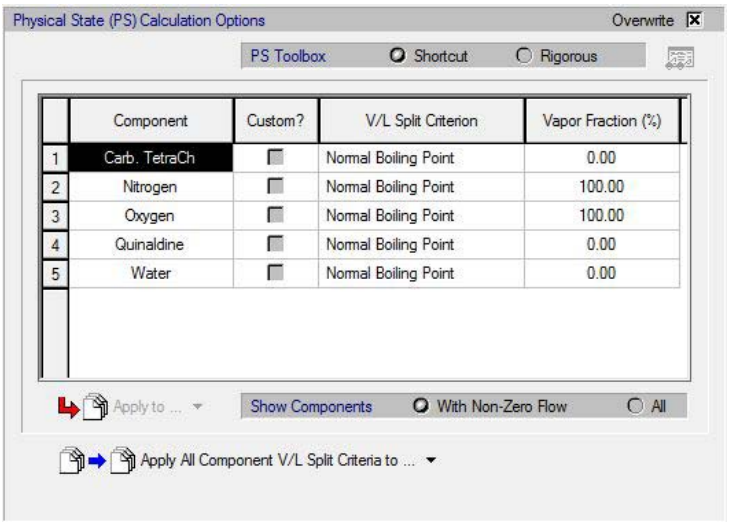


Figure 5.12: The Physical State calculation options tab for a bulk stream.

- By selecting a component with a *customized* V/L split criterion and pressing the button, the following options become available: to all components by clicking the button, the following options become available every other
-

.

By alternating between the Show Components With Non-Zero Flow and All options, you can prevent the components that are not actually present in a procedure state from being displayed.

▶ How to customize the Rigorous Toolbox options for one or more procedure states in a procedure...

1. While in select mode, right-click on the procedure icon and select **Procedure State Options...**.
2. Visit the respective tab of the procedure state whose PS calculation options you would like to change. Please remember that each tab represents the state of the procedure (a.k.a., equipment contents) right *after* the operation mentioned at the top of the tab.
3. Check the Overwrite checkbox in the Physical State (PS) Calculation Options frame.
4. Make sure the Rigorous Toolbox option is selected.

5. Click on the Edit Rigorous Toolbox Options button .
6. In the Rig. Toolbox dialog that appears (Figure 5.13), specify the desired VLE model from the K-value calculation model drop-down list (see 8.12b The Rigorous Physical State Calculation Toolbox for more details).

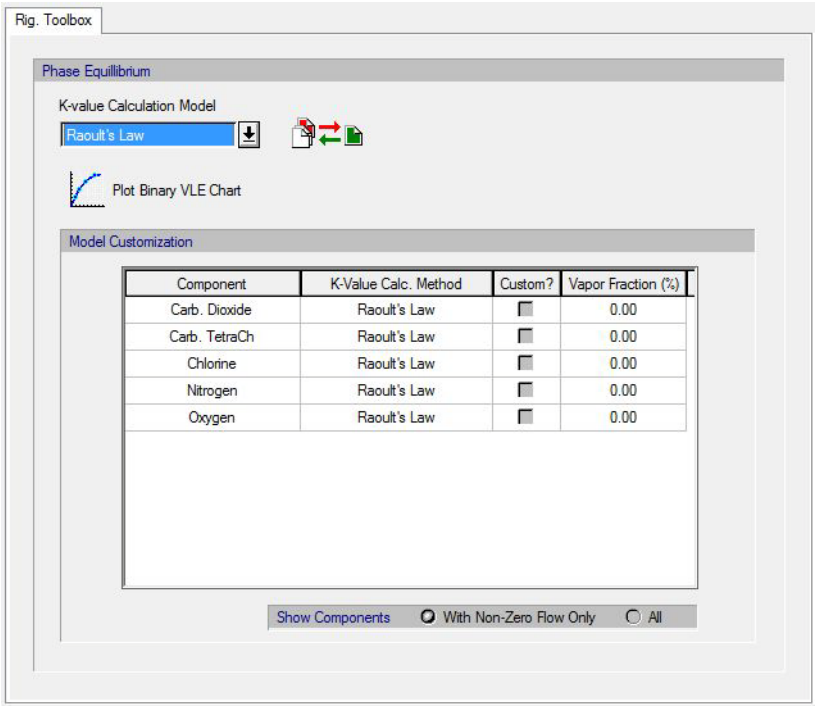


Figure 5.13: The Rigorous Toolbox dialog.

5.12b Procedure State Density Calculation Options

For each procedure state, SuperPro Designer calculates the individual densities of the liquid/solid and vapor phase (see 8.13 Density Calculation Options) as well as the total density of the procedure state. By default, every procedure state is initialized with the density calculation options of the procedure that they belong. Of course, all such procedure density modeling options originally are inherited from the settings chosen for the entire process. Users may intervene at any point and engage a different model in the calculation of phase densities. The can change the liquid/solid and/or vapor density model at the procedure level by selecting **Default PS Calculations...** from that procedure's command menu.

It is possible to deviate from the default settings for the calculation of density in one of the following ways:

1. Modify the liquid/solid density calculation options

2. Modify the vapor density calculation options

When the Overwrite check box is checked, the density calculation options for that procedure (and all its states) become independent of the respective options of the process file. As a consequence, possible changes in the density options of the process file will not be propagated to the procedure states.

In the ensuing dialog, after checking the "Overwrite" box for either the Liquid/Solid Phase or the Vapor Phase (or both) the user can enforce a new model for that phase. Any changes made there will automatically be applied to all contained procedure states. In a similar way, a user may chose to part with the procedure density calculation options at a specific procedure state. This can be done by selecting the **Procedure State Options...** from the procedure's command menu. Then, navigate to the desired procedure state and make your new choices after the "Overwrite" check box is marked where appropriate. Note that each tab represents the procedure state (a.k.a. equipment contents) after the operation named at the top of the tab is executed. Once the "Overwrite" box is checked, any future changes in the procedure's settings will *not* be propagated to that state.

CUSTOMIZING THE DENSITY CALCULATION OPTIONS OF PROCEDURE STATES

▶ How to overwrite the Density Calculation Options...

1. While in select mode, right-click on the procedure icon and select **Procedure State Options**.
2. Check the respective Overwrite checkbox for the Liquid/Solid or Vapor Density (Figure 5.14).
3. Make the desired changes regarding user-set density values, volumetric coefficients, etc.

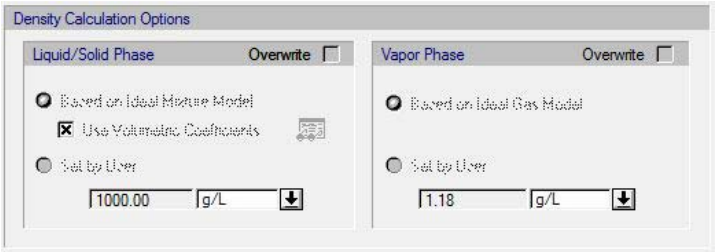


Figure 5.14: The procedure state's density options.

5.13 PROCEDURE PS AND DENSITY CALCULATION DEFAULT OPTIONS

Each procedure in a process file has its own set of default options for the Shortcut and Rigorous toolbox *as well as a default selection regarding which one of the two toolboxes will be used* for the calculation of the physical state of material. These default options are automatically propagated to all of its procedure states and associated output streams unless the Overwrite

option has been enabled for any of them. A detailed description of the physical state calculation options is given in 8.12 Physical State Calculation Options.

By default, every procedure in the process is initialized with the Shortcut PS Calculation Toolbox. It is possible to change the default settings at the procedure level by modifying the assigned PS Toolbox selection as well the respective PS Toolbox options.

In addition, every procedure has its own set of default options for the calculation of liquid/solid and vapor density. By default, every procedure state is initialized with the density calculation options of the process file (unit procedures do not keep a set of default options for density calculations) and any change to the options of the process file will be propagated to the procedure . It is possible to deviate from the default procedure settings for the calculation of density in one of the following ways:

1. Modify the liquid/solid density calculation options
2. Modify the vapor density calculation options

CUSTOMIZING THE PROCEDURE PS CALCULATION DEFAULT OPTIONS

1. While in select mode, right-click on the specific unit-procedure and select **Default PS Calc. Options**
2. Check the Overwrite checkbox in the Physical State (PS) Calculation Options frame.
3. Select between the Shortcut or Rigorous PS Toolbox option and if necessary, modify the respective PS Toolbox options in the same way as for the individual Procedure States (see Procedure State Physical State Calculation Options).

RIGOROUS TOOLBOX-ONLY UNIT PROCEDURES

The following 4 unit procedures essentially require by nature the Rigorous PS calculation toolbox to carry out the modeling calculations of their respective operations.

Flash	Select **Procedures ▸ Phase Change ▸ Flash**
Rigorous Distillation	Select **Procedures ▸ Distillation ▸ Rigorous**
Condensation	Select **Procedures ▸ Phase Change ▸ Condensation**
Thin-Film Evaporation	Select **Procedures ▸ Phase Change ▸ Thin-Film Evaporation**

In these unit procedures, the Shortcut toolbox is not applicable and the Rigorous toolbox is employed as the only option..

For the Rigorous toolbox-only procedures the PS toolbox options coincide with the respective options of the associated operations.

The physical state of streams coming out of Rigorous toolbox-only procedures is determined by the procedure itself. For example, the top output stream of the Flash procedure is considered to be exclusively in the vapor phase while the bottom stream is considered to be exclusively in the liquid phase.

The physical state calculation options of such streams cannot be overwritten (see Figure 5.15). This is done purposely to avoid energy balance inconsistencies (i.e., the creation or loss of enthalpy content on a stream) due to the discrepancy of the PS calculation options between the unit procedure and its associated output streams.

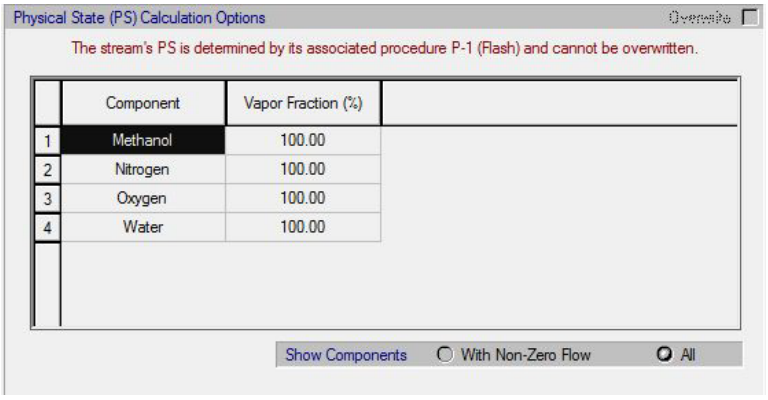


Figure 5.15: The PS calculation options of output streams of a Rigorous-toolbox only procedure.

CUSTOMIZING THE DEFAULT PROCEDURE DENSITY CALCULATION OPTIONS

1. While in select mode, right-click on the procedure icon and select **Default PS Calc. Options.**
2. Check the respective Overwrite checkbox for the Liquid/Solid or Vapor Density (Figure 5.16).
3. Make the desired changes regarding user-set density values, volumetric coefficients, etc.

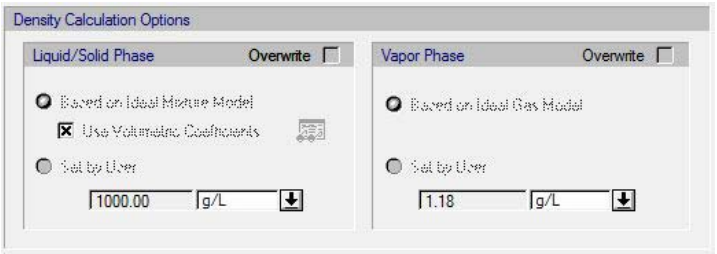


Figure 5.16: The procedure default density options.

5.14 DEFAULT DATA VALUES FOR INPUT VARIABLES

When you open the i/o simulation dialog for a newly created operation you may be surprised to see values be displayed for some of the variables that are required as inputs. These values reflect typical operating conditions. Having such default values is very convenient, especially in cases where you are about to simulate an operation for which experimental data are not readily available (for your specific application). However, caution should be exercised when evaluating the outcome of a simulation (or an economic evaluation) that is based on such default values, without any knowledge of the range of the actual parameters in your specific industry.

SuperPro Designer requires that you visit each of the i/o simulation dialogs for all the operations involved in a process. If you attempt to execute the mass and energy balances in a process that includes operations which have never been initialized you will get the following error message:

“Operation <name> has not been initialized yet, or needs to be re-initialized.”

If that appears, you need to visit the i/o simulation of the above operation. Please note that when you attempt to close the i/o simulation dialog of an operation, SuperPro Designer checks all values (as shown at the time) to make sure that they are within the allowable range, and consistent with other settings (on the same operation or elsewhere).

1.
2. Comments Sign: Displays an indicator () at the bottom-right of the unit procedure icon, when the equipment, procedure or any operation contains comments.
3. Equipment Allocation Label: Displays a label with information regarding the equipment allocation (see

6

RESOURCES

During the running of a process there are several types of resources that are engaged. Such resources are either consumed and therefore add a cost penalty to the operating expenses of the process (e.g. raw materials, power, heat transfer agents) or are simply employed (e.g. equipment units, labor units) but due to limits of their availability they may present bottlenecks to certain process configurations. We are going to describe in detail all the resource types that can currently be represented by SuperPro Designer and show how these resources are associated with functional elements of a process as well as how their consumption is tracked, viewed and reported. The application recognizes the following as resources:

1. Equipment (Main & Auxiliary), see 6.1 Main Equipment and 6.3 Auxiliary Equipment.
2. Materials, see 6.5 Materials.
3. Heat Transfer Agents, see 6.7 Heat Transfer Agents.
4. Labor, see 6.11 Labor.
5. Power, see 6.9 Power.
6. Storage Units (Supply & Receiving), see 6.13 Material Storage Units.

For each resource, the application will present charts displaying exactly how they are engaged (or consumed) during the span of a single or multiple batches. Since batches may be set to have a partial overlap during execution, it is important to study the effects of stacking up batches as most bottlenecks in resource utilization will appear during that period. For storable resources (such as materials), SuperPro Designer can also perform an inventory analysis if the user provides information related to the replenishing of the resource. Special charts (inventory charts) can be presented that combine the consumption side as well as the replenishing side of such resources thereby allowing the user to design properly holding containers and/or capacities for the replenishing (or restocking) process.

When studying resource consumption (or inventory) in multiple batch scenarios it is important to remember that SuperPro Designer will always assume a perfectly orderly production of batches, always spaced apart by the same amount of time (process cycle time) and always repeating the exact same sequence of events for each batch (shifted properly in time). In other words, the user cannot schedule each batch as a whole or the events in each consecutive batch individually. Therefore, any such analysis cannot address irregularities (expected or unexpected) that may occur between batch executions. To address such concerns users should consider exporting a SuperPro Designer process to SchedulePro (Intelligen's complementary product that addresses such concerns most efficiently).

6.1 MAIN EQUIPMENT

Almost all unit procedure types assume that the operations set to execute in their sequence order are carried out in a host equipment resource (the' Transportation' and the 'Design Spec' procedures are the only exception and have no host equipment). The name of the equipment resource associated with a unit procedure is, by default, displayed as part of the name label under the procedure's icon. The actual type of equipment resource is automatically selected by the program once a procedure type is selected. For example, once you select to introduce a new condensation procedure (under **Unit Procedures ▸ Phase Change ▸ Condensation**), then click on the worksheet the new procedure is automatically assigned an equipment resource of type 'Condenser' with the name 'HX-101'. As soon as a new procedure is created, SuperPro Designer always creates a new equipment resource behind it. You can customize the prefix ('HX-') and the default numbering scheme used by the application when composing the name of new equipment resources (see 8.20h Automatic Name Generation).

*Do not confuse the pictorial view of the icons on the flowsheet (they look like equipment units) with their representational meaning: they represent processing steps and not equipment. We have made the procedure icons reminiscent of their hosting equipment resource types in order to better convey visually the unit procedure type of each icon. Since equipment resources are not directly represented on the flowsheet, the unit procedure icon represents the graphical user interface gateway to addressing the equipment resource behind the procedure. That is why the command menu (right-click menu) of a unit procedure contains entries related to data about the equipment hosting the procedure (**Equipment Data**, **Equipment Contents**., etc).*

EQUIPMENT FEATURES

It is possible to have two procedures of the same type (e.g. Storage in a Disposable Large Bag) be displayed by icons that may be slightly different. The difference in the iconic representation of the procedures may be due to a different set of **equipment features** that may be selected for the respective equipment resources. For example, one of them may be set to allow for heating/cooling exchange to happen with a heat transfer agent whereas the other may be set to allow for continuous stirring. Such equipment features (if available) are always selected from the first property page of the Equipment Dialog. Besides dictating the specific icon displayed for that procedure, a feature set may also dictate the availability of certain operations in the hosted procedure(s). For example, if a heating/cooling jacket is set to be available, then "Cool" and/or "Heat" may be an operation choice, but if this feature is not selected, then they may not be available.

6.1a Equipment Sizing (Design vs Rating Mode)

When assigning an equipment resource to a newly created procedure, the program assumes that the size of the engaged equipment resource is not known. As part of the simulation calculations, the application will also size the equipment resource so that it can accommodate the needs for capacity (or throughput) of the most demanding amongst the operations included in the procedure. For example, as we charge more and more material in a vessel the needs for capacity keep increasing. the program will keep track of the demand and at the end of the procedure it will size the equipment such that it fits all of the charged material. When the equipment resource is set to be sized by the program, we call it being in **Design Mode**. On the other hand, when the user already knows the size of the engaged equipment resource (e.g. he/she knows that the hosting vessel has a given capacity or size dimensions) then, he/she

needs to switch the equipment to **Rating Mode**. When in this mode, the dimensions (or other related size specifications) of the equipment resource are available for editing in the equipment dialog and should be provided by the user. The choice between design vs rating mode can be made from the Equipment tab of the Equipment Dialog. Even though the entire arrangement of the tab depends on the specific equipment resource type (Vessel, Filter, Chromatography Column, etc.) the left side of all interfaces is always the same (the Equipment Data Dialog: Equipment tab). When the equipment is being sized by the application after the mass and energy balance calculations (i.e. it is set to design mode) there will always be a variable that provides an upper limit on the size, in order to keep the actual sizes realistic. For example, when sizing a vessel, the user must always provide a maximum volume; when sizing a membrane filter, the user must provide a maximum membrane area. If the size that is required to accommodate the operations hosted by the equipment exceeds the maximum value, then SuperPro Designer will assume the presence of multiple pieces of equipment, all with identical sizes and within the available range. This multiple number of units are shown on the equipment dialog as 'Number of Units' and they are assumed to operate in parallel when the equipment host is engaged. When the equipment is in rating mode, this field is open and can be set by the user.

6.1b Equipment Selection & Sharing

In batch processing, in order to make best use of equipment resources that may be sitting idle, it is quite common to have more than one processing steps (that are part of the same batch or different batches) execute in the same hosting equipment. Very commonly, storage vessels are used to hold outputs from various steps of the process until the next step processes the material. Also, filtration units or chromatography units may be utilized during various stages of the batch. Sharing of equipment across batches can also be feasible, which means equipment can be utilized by the same processing steps at different instances of the same batch. Clearly, such reuse saves on extra equipment but at the same time imposes a constraint on the times that each of those procedures may be carried out since their engagement times cannot overlap.

▶ **To share a main equipment resource between two procedures…**

1. Create the two procedures (e.g. P-1, and P-2). Each one will be assumed to have its own (new) equipment resource (e.g. V-101 and V-102).
2. Visit the Equipment Data Dialog of the second procedure (by selecting the **Equipment Data** option from the procedure's command menu).
3. At the top left corner of the Equipment Data Dialog: Equipment tab, select (from the drop-down list) the name of the first equipment resource (V-101), and click **OK**.

In general two procedures of the same type are assumed to be hosted by the same type of equipment resource and therefore they can be made to share a common equipment instead of each one utilizing its own. However, if the equipment resource is characterized by features (see Equipment Features) then in order for a procedure to be allowed to relinguish its own equipment and assume the equipment of another procedure (of the same type), the operation list must also be compatible with the feature set of the surviving equipment resource.

In cases where more several procedures share the same equipment resource, the application

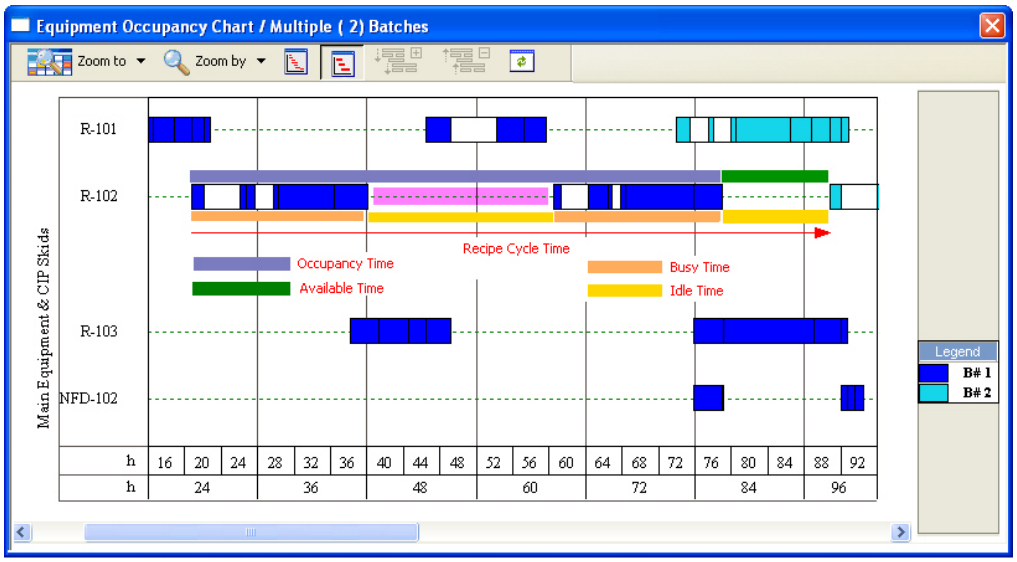


Figure 6.1: A sample equipment occupancy chart.

displays several time measures that can gauge how efficiently the resource is being utilized within the same batch as well as across batches. To better understand the utilization of an equipment resource, the following terms need to be defined (please refer to Figure 6.1 showing an equipment occupancy chart for a sample process):

Procedure Occupancy Time: The time elapsed between the start and the end of a procedure hosted by an equipment resource; if the procedure is set to execute in multiple cycles, then it is the time between the start of the first cycle and the end of the last cycle of that procedure.

Waiting Time: The sum of all the time intervals between the end of a procedure and the start of the next procedure (hosted by the same equipment resource) as part of the same batch.

Idle Time: The time that the equipment resource is not hosting a procedure (per batch). It includes the waiting time plus the time between the end of the last procedure in a batch and the start of the first procedure as part of the following batch.

Busy Time: The sum of all the procedure occupancy times; it represents the time that the equipment is active (busy) during a batch.

Occupancy Time: The time spanned from the start of the first procedure to the end of the last procedure of the same batch. It may include spans of time that the equipment is idle as it is waiting for the next procedure (of the same batch) to start executing. By default, it is assumed in SuperPro Designer that an equipment resource cannot be employed for a future batch until all uses for the current batch are exhausted. If an equipment is allowed to be employed in a future batch before all the procedures of the current batch have used it, then the occupancy time is equivalent to the busy time of the equipment (see also 7.3 Scheduling Calculations).

Unoccupied Time: The time that the equipment is not considered occupied during a batch. It is essentially the complementary time to the occupancy time (i.e. the sum of occupancy time and

unoccupied time is the recipe cycle time or time between consecutive batch starts). It is essentially the time that an equipment resource waits until it is engaged by the next batch.

The terms 'Occupancy Time' and 'Unoccupied Time' have only meaning when viewing the equipment resource in a multiple batch perspective. Clearly if an equipment is not used across batches it is only truly occupied during the execution of a batch when each of the hosted procedures are being carried out and not during its waiting time.

The above measures for a given equipment and/or procedure are shown on the equipment dialog or the procedure dialog (respectively). To gain a general overview of how all of your equipment is being utilized during a process in a chart or a table format, please select **View ▸ Main Equipment Occupancy Data ▸ Table** to display the Main Equipment Occupancy Data Table or **View ▸ Main Equipment Occupancy Data ▸ Chart**. to display the Main Equipment Occupancy Data Chart.

EQUIPMENT USE ACROSS BATCHES

There are cases when an equipment resource may be used by several procedures (during the span of a batch) but there may be long periods of time between each such utilization. Normally, during the long idle in-between-usage time, SuperPro Designer considers the equipment 'occupied' (to preserve batch integrity) and does not allow any follow-up batches to engage it. If a user didn't care for batch integrity, he/she could allow a designated equipment to be used by a procedure of a follow-up batch before all utilizations of the current batch ended. This practice may lead in better overall equipment utilization but at the expense of increasing the possibilities of equipment sharing violations. In order to allow the program to utilize an equipment resource in this manner, you must check the "Allow Use Across Batches" flag in the Equipment Data Dialog: Scheduling Tab. Obviously this option is only meaningful for equipment which is shared by more than one procedures. As this tighter integration of equipment utilization can lead to more situations where equipment violations may occur, we need to have a much more sophisticated algorithm that predicts which cycle time result in such violations. SuperPro Designer has such algorithm that can produce the cycle time windows that avoid sharing violations (see Scheduling Constraints). The Cycle Time Bounds Calculation can be triggered from the Recipe Scheduling Information Dialog.

6.1c Staggered Mode

As explained in detail in the scheduling calculations (see 7.3 Scheduling Calculations) the cycle time of a process cannot be lower than the longest occupancy time amongst all equipment involved. When the occupancy time of an equipment resource is too long (compared to rest of the equipment) it forces a very long time between consecutive batch starts and therefore it introduces a much undesirable under-utilization of a the rest of the equipment in the process. For example, when modeling a fermentation process the fermentation itself could take a week, when all the downstream purification steps don't take more than several hours. If we had to wait till the fermentor becomes available before we start a second batch, then clearly we couldn't start a batch for a week at a time. Notice that while the fermentor would be busy for a week the rest of the equipment would be idle for 6+ days. To avoid such undesirable utilization of process equipment, we can request the equipment resource behind fermentation to involve 6 extra sets of units operating in **staggered mode**. This will reduce the 'effective' equipment occupancy time for the fermentation step from 7 days to 7 / (6+1) = 1 day. Now, the calculated

minimum cycle time will be 1 day and by starting a batch every day we also make best use of the rest of the equipment.

You can request a staggered mode for an equipment resource from the Equipment Data Dialog: Equipment tab.

If the number of units for an equipment is set (or calculated) to be more than one, then when turning on the staggered mode for a given equipment resource, the application must assume that for each shift of the staggered equipment there must be an equal number of units operating in parallel. Note that these extra units will add to the capital cost of the process.

The extra staggered units will be given names constructed from the name of the original equipment plus the "STG01 >>", "STG02 >>" prefix. If you wish to provide your own names you can do by visiting the Equipment Data Dialog: Purchase Cost Tab names dialog that is accessible from the Equipment Data Dialog: Equipment tab.

6.1d Contents

Many equipment resource types have a volume property and as such, they are capable of holding material during the execution of a unit procedure (e.g. a vessel or a nutsche filter). When a procedure executes in such equipment, SuperPro Designer keeps track of the equipment contents before and after the execution of each operation. It is assumed that at the beginning of the batch, each such equipment holds some material (**initial equipment contents**). By default, the application assumes that all such contents are just air. However, if needed, the user can provide a new strategy for initializing the contents before first use in each batch. Besides the default initialization the other choices are three:

1. Initial contents are directly specified by the user.
2. Use as initial contents whatever was left by the previous simulation run.
3. Auto-initialize initial contents by copying the material contained in another equipment (in the same process file or in another process file).

The strategy #2 above (or more precisely a combination of #1 and #2) may be useful in cases where a vessel feeds the process with material that is supposed to come from a later step in the process (in other words, there's a recycling loop in the process). If you don't chose to represent the feeding and receiving operations together in one procedure (thereby forcing a real loop on the flowsheet that requires iterative calculations to be solved) then, the composition and amounts of material in the equipment resource will change from simulation to simulation until they eventually converge to a stable value. Furthermore, the initial amount in the vessel (to be used during the first simulation run) must be set by the user. Strategy #3 may be useful in cases where a rather large process is broken down to smaller, simpler steps each modeled as a separate process file. In that case, one may wish to initialize the contents of a given equipment that holds material at the beginning of a step, with whatever was left at the end of the previous step (through the Initial Equipment Contents: Initialization Options Dialog). Note that this linking between files can also be accomplished by associating the contents of an input stream in a flowsheet with the contents of another stream in another process file (see 4.9 Auto-Initialization of Input Streams).

The choice for initial content strategy can be set from the Initial Equipment Contents: Initialization Options Dialog that appears when selecting **Equipment Contents ▸ Initial ▸ Options** from the procedure's context menu. If you decide to provide your own composition

and amount, then you must visit the Initial Equipment Contents (View/Edit) Dialog by selecting **Equipment Contents ▸ Initial ▸ Edit** from the procedure's context menu.

You can view the equipment contents during the execution of a procedure using the Equipment Contents Dialog that appears when you select **Equipment Contents ▸ During <Procedure Name>** from the procedure's context menu. If more than one procedures are hosted by the same equipment resource then selecting **Equipment Contents ▸ During All Procedures** will show the Equipment Contents Dialog displaying the contents of the equipment during the entire sequence of execution of all procedures.

If the equipment resource is deployed by more than one number of units, the equipment contents shown indicate the amounts held collectively by all units. If the procedure is set to execute in multiple cycles, then the amounts shown before and after each operation correspond to the equipment contents after the execution of the first cycle.

6.1e Local Receptacle & Automatic Emptying of Contents

Since equipment resources can be reused in the span of a single batch, most of the times the follow up procedures utilizing an equipment resource do not expect to find any material in it. To make sure that when a procedure takes over the use of an equipment resource it never inherits any contents from the previous procedure (regardless of settings or conditions during the execution of the operations in the previous procedure), then you must activate the automatic emptying of contents feature. When this equipment feature is turned on, before a unit procedure engages the equipment, a check is being made: if any liquid material is found as leftover from the previous procedure that utilized the equipment, it is removed and placed in a local receptacle (not shown on the interface). If the same conditions exist before the second reuse of the equipment, then the liquid leftovers after the second use will also be emptied (and mixed) to the local receptacle.

The activation or deactivation of the automatic emptying before reuse of the equipment can be made from the Empty Contents Before Reuse Dialog that appears when selecting the **Equipment Contents ▸ Before Reuse ▸ Emptying to Local Receptacle** option from any procedure (that uses the equipment) command menu. From the same dialog, the user will also have the chance to classify the waste as well as provide a disposal cost and (if needed) a collection storage unit.

After the conclusion of the M&E balance calculations, you can view the contents of an equipment's receptacle by selecting **Equipment Contents ▸ Before Reuse ▸ View Receptacle Contents** from any procedure (hosted by the equipment) command menu.

6.1f Purchase Cost

A very important component of the economic expenditure especially for new (green field) projects, is the total capital cost for the equipment necessary to carry out the process. SuperPro Designer has built-in models that estimate the cost for each equipment type based on its size variable. As some of the formulas used for the cost estimate have been given to us by manufacturers we do not publish them. However, if you do not agree with the program's estimates, you can either provide a fixed value for the specific (as sized) equipment or supply your own cost vs size model that will be used to estimate the cost given the value of the sizing parameter. We call this model the **User-Defined Cost Model** or **UDCM** for short.

If you have allocated the equipment resource to a database equipment, see 6.1i Equipment Allocation, then its purchase cost is read from the database and no other choice exists for its estimation.

All built-in models for cost estimation produce the cost in US$ at a given year. The cost is brought up to the project's date by adjusting for inflation using the published Chemical Engineering Index. When specifying your own UDCM you also need to specify the year for which the estimates are valid. If the project year is different then the costs will be adjusted the same way.

THE USER-DEFINED COST MODEL (UDCM)

This model can be provided by a user as a cost vs size correlation that will be used by the application to estimate the cost of a piece of a equipment if the built-in model produces unacceptable results.

The general formula used for the model is a power-law type: $C = Co\ (Q/Qo)^a$

where, (Co, Qo) is a pair of reference size and cost, and a is an exponent (usually less than 1).

The user is supposed to provide the triplet of (Co, Qo and a) as well as a range of size values (Q) where the triplet of values generates a valid estimate. Note that if it is not possible to have a single triplet of values for the entire range of expected sizes (Q), then you can divide the entire range into smaller segments and provide a different set of triplet for each range. Please note that the variable used to feed the cost vs size UDCM is fixed for a given type of equipment resource. The units can be changed but will always be of the same units type as the variable. For example, for vessels the size is expected to be the volume of the vessel in volume units; for a plate-and-frame filter, the UDCM is supposed to estimate the cost as a function of the filter area in area units. Also, it is assumed that the cost estimate is in currency that is (at the time) selected as the chosen currency for the current process file (see 9.8 Currency). As part of the UDCM definition, the user is supposed to provide a year for which the cost estimate is valid. SuperPro Designer will update the cost to the current year that the project is carried out by using the chemical engineering index to account for inflation.

User-defined cost models may be also imported from the database. These UDCMs have been either defined in the User Defined Cost Models Databank or were first introduced in equipment of the process and then deposited into the database for safe keeping and/or for re-use in other equipment of the same type.

When specifying the UDCM for an equipment resource, it only applies for the specific resource used in that process step (unit procedure). It does not replace the cost estimation option used for all equipment (of similar type) employed by your process. If you wish to use the same cost model for all equipment of the same type, then you must either specify the same model in all other equipment present in your process (one-by-one), or specify the UDCM in the first instance of the equipment and then copy-and-paste the procedure/equipment pair before you use it elsewhere in your process. Additionally you may also deposit the UDCM from an equipment in the database and then import it back into the process to which ever equipment of the same type it is needed.

For more information on the user-defined cost model interface see User-Defined Cost Model Dialog. Also all of the above choices and parameters including the UDCM interface can be viewed and/or edited through the Equipment Data Dialog: Purchase Cost Tab.

6.1g Cost Adjustments

After the base purchase cost for the equipment is estimated there are several other equipment parameters that can affect either the final purchase cost of the equipment or other aspects of the direct fixed capital (DFC) of the section that the equipment belongs (e.g. installation), or even the facility component of the operating cost.

PURCHASE COST ADJUSTMENTS

Material Factor: The base purchase cost is estimated assuming a default material of construction (the actual material may vary from equipment to equipment but typically it is SS316). To adjust for construction requirement with special needs, other materials and material construction factors can be defined for a given equipment type. If you wish to introduce a new material of construction along with its material factor you should visit the Equipment Materials Databank (see15.11 Equipment Materials Databank). The material factor is supposed to scale the cost up or down in relation to the base cost. If no material factor exists for one of the existing materials (or even if it exists but you wish to overwrite it), then you can specify a value in the Equipment Data Dialog: Adjustments Tab.

Standby Units: For pieces of equipment that can be critical for the operation of the process, you may choose to have one or more extra pieces as standby (in case the regularly used pieces of equipment go down for scheduled or un-scheduled maintenance). The extra units are assumed to be of the same size (and cost) as the main units.

Installation Factor: It is used to provide an estimate for the installation cost as a multiple of the purchase cost.

PC Portion Allocated to This Project: If the equipment participating in this process may be purchased with the intention to be shared by other projects, then it is customary for the equipment purchase cost burden to be split between the two (or more) projects. Any value less than 100% will reduce the capital cost contribution of this equipment resource to the section's DFC. Note that any PC-derived quantities (such as installation or maintenance) will still be using the full value of purchase cost.

OPERATING COST ADJUSTMENTS

Maintenance Cost Factor: A multiplier to be used in conjunction with the equipment's capital cost to estimate annual maintenance.

Usage & Availability Rates: If the facility component of the operating cost is estimated directly from usage & availability rates, then these factors will provide the charges associated with this equipment. Note that usage rate is based on the actual occupancy time of the equipment, whereas the availability rate multiplies the entire time the equipment is dedicated to this process (and therefore it includes idle time).

Portion of PC Already Depreciated: This factor if set to anything other than 0, reduces the portion of the equipment's PC that will be used to estimate the annual depreciation. It should be noted that this factor will only affect the amount of depreciation calculated and not the actual contribution to the DFC due to this equipment. Furthermore, any PC-dependent quantities (like installation, maintenance etc.) will still be based on the full value of purchase cost.

All of the above variables are viewed and/or edited through the Equipment Data Dialog: Adjustments Tab.

6.1h Consumables

Consumables are items that are used by equipment in the process for few times and then they are disposed. Examples of consumables may be filter cartridges, chromatography resins, etc. Some equipment need to have such consumables present so that they function properly. These consumables are called **required consumables** and the equipment types that need them have dedicated variables (and interface) that lets the user view their properties (type, replacement rates, etc.). On the other hand, every equipment has the potential of being assigned the consumption of some generic consumable that may be needed in a given situation. For example, some machinery may require frequent lubrication (e.g. grinders) or cleaning power. If you need to employ a particular consumable that is not currently available, then you must first introduce it in the Consumables databank through the Consumables Databank Dialog. After the consumable has been defined, then you can associate it and define its usage rate to a specific equipment from the Equipment Data Dialog: Consumables Tab. A key variable needed for each consumable use associated with an equipment resource is the consumption rate (how much of the consumable is needed per use) and the replacement frequency (how often the consumable is disposed of). Once a consumable is specified for some equipment in your process file, that consumable will also be included in the Consumables Currently Used by the Process Dialog for that file.

6.1i Equipment Allocation

Equipment resources in a process can be allocated to **site equipment** or they can simply be matched to a **vendor equipment (equipment spec sheet)**. Allocating an equipment resource is essentially a commitment to use for the given resource an actual piece of equipment (owned or leased) that is available in a manufacturing site. Having equipment resources bound to either site equipment or vendor equipment provides the benefit of consistency across different process representations within a corporation.

Matching an equipment to a vendor's equipment specification sheet (aka vendor equipment) is essentially a commitment to use the specific vendor as source and the specific vendor's model when the time comes to purchase the equipment unit(s) needed for the given equipment resource. If a company always prefers to use a certain line of dead-end filters from a given vendor, then all engineers that employ dead-end filters in their process description can match such equipment resources to the specification sheet with size that matches the need of their process and from then on, the actual size and the cost will be shown precisely as expected. Vendor equipment specification sheets can be defined (and made available to all users of SuperPro Designer) in the equipment from vendors databank (see Vendor-Equipment Databank Dialog).

Descriptions of manufacturing sites along with resources that may contain (equipment, heat transfer agents, labor, etc.) can also exist in the user's database in the form of **database sites**, (see Sites & Resources Databank Dialog). Once again, once those sites are populated, other users of the application can allocate the resources employed in their process simulations to the database objects to ensure consistency.

Regardless of whether you chose to match an equipment resource to a vendor equipment or allocate the equipment resource to a site equipment, once the connection is made, then all size properties (e.g. volume, diameter, height etc.) and the purchase cost of the equipment is read from the database and 'frozen' in your process description. If you visit the equipment data dialog, the first tab ('Equipment') will show the description of the equipment (on the right-hand

side) with all the size fields frozen. Also, the sizing option for the equipment (shown on the left side of the same tab) will always show as rating mode and also frozen (so you are not able to switch to design mode).

The option for allocating an equipment resource to a site equipment is only available if the process section that the specific equipment resource belongs, has been already allocated to a database site.

To allocate a section to a database site, you must visit the Section Properties Dialog: Allocation tab. To allocate an equipment resource to a site equipment, you must visit the Equipment Data Dialog: Allocation Tab.

6.1j Vendors, Vendor Equipment & Type Specification Variables

Process equipment in a SuperPro Designer process can be matched to an equipment specification sheet as stored in the user database. In order for a company to make consistent use of equipment throughout its organization, the program lets you define in the user database a list of vendors and equipment specifications that are the preferred choices for the organization. When submitting a specific equipment model, SuperPro Designer expects you to provide at least two pieces of data: size and cost. However, for you own documentation and in order for your users to understand better the choices available, you may want to describe a vendor's equipment model with more attributes. SuperPro Designer allows you to introduce your own (new) set of attributes and attach them with their appropriate values to your vendor equipment specification records. For example, you may want to describe the type of automation or the type of instrumentation included in a given model, or the time availability for certain models.

To introduce vendors, vendor equipment, and variable types, you must visit the Equipment Vendor/Manufacturer Databank Dialog, the Vendor-Equipment Databank Dialog, and the Equipment Types & Specifications Dialog, respectively.

6.1k Equipment Type Categories

Whenever you view equipment types in SuperPro Designer, they are always organized in groups. Each group contains a set of equipment types that are of some common nature. You can view the all equipment types currently recognized by the application when browsing the equipment types databank (**Equipment ▸ Types & Specifications**). Similar organization of equipment types exists in the equipment tab of the Process Explorer Toolbar. The same set of groups appears as top nodes in the equipment prefix customization tab (Application Settings Dialog: Prefixes tab). The same tree-like organization appears when selecting an equipment type in the site-equipment databank (select menu **Databanks ▸ Equipment ▸ in Sites**) or vendor-equipment databank (select menu **Databanks ▸ Equipment ▸ from Vendors**).

6.2 MAIN EQUIPMENT CHARTS & TABLES

Since equipment resources are so important, especially for batch processes with long recipe times, the application offers the user a multitude of charts and tables with information on how equipment is being utilized in the span of a single or multiple batches. Probably the most important chart for equipment use is the Equipment Occupancy chart as it visually conveys for

each equipment its utilization. The multi-batch version of the chart is especially important as it directly shows the equipment scheduling bottleneck for the process. The Equipment Gantt chart offers the same information as the occupancy chart, only in a Gantt-chart format, where each occupancy bar is expanded (in a separate line) to its details. Other tables & chart focus on the occupancy measures (indices) for each equipment resource (see 'Occupancy Indices' on page 6-17).

6.2a Equipment Occupancy Chart

To bring up the chart for a single batch, select **Charts ▸ Equipment Occupancy ▸ Single Batch** from the main menu; selecting **Charts ▸ Equipment Occupancy ▸ Multiple Batches** from the main menu will bring up the chart for several batches. In a continuous process that contains batch procedures select **Charts ▸ Equipment Occupancy ▸ Selected Time Horizon** from the main menu.

Each y-entry represents a main equipment resource and/or an auxiliary equipment resource (such as CIP, SIP etc.). You can customize the contents (e.g. if you wish to view the main equipment only) by changing the chart's style (through the Graph Style for Equipment Occupancy Data Chart interface). The visual appearance of the occupancy bars (aka task bars) can also be customized (for single batch charts) from the chart's style. The equipment appear in an order that can also be customized (if so desired). By default, the equipment resources are ordered by time of engagement (earliest at the top to latest at the bottom). If you wish to overwrite the default order then you may select **Include ▸ Exclude ▸ Order Equipment** from the chart's command menu or from the Equipment Occupancy Data Chart Style Dialog: General tab.

DEFAULT NUMBER OF BATCHES

When a multi-batch chart is chosen to be shown, the default number of batches (N_b) shown at first is calculated as follows:

$N_b = 1 + [BT / CT]$, where

[BT/RCT] is the rounded up integer ratio of the recipe's batch time (BT) divided by the recipe's cycle time (CT). The number is chosen this way, so that even if you later view a larger number of batches, all future batch graphs will always have a pattern that can be mapped within this chart (with some offset). In other words, N_b as calculated above, is the minimum number of batches necessary to plot such that it will capture all possible batch interactions. Of course the number of batches can later be set to any number (select **Set Number of Batches** from the chart's command menu). Optionally the time horizon can be set and therefore the number of batches will be adjusted so as to fit the selected time span.

SuperPro Designer uses a default coloring scheme for presenting all the occupancy bars belonging to the same batch. This makes it very easy to visually convey the batch number for each activity (task) bar. The legend window at the side of the chart indicates which color has been chosen for each batch ID. The user can modify the color to be used for a given batch ID by simply double clicking on its color sample in the legend window.

TIME LINE

The x-axis represents time. By default, the axis start time is 0.0. In other words, the time value of 0.0 is assigned to the earliest engagement of an equipment (aka beginning of the batch). If so desired, a real date/time can be assigned through the Graph Style Dialog (All Time Charts):

Time Line Tab. The time axis displays two lines with increments of time: minor and major. The settings for what time increment to be used for major and minor increments as well as what units to be displayed is also customizable. By default a vertical gridline will be displayed on both minor and major increments but they can be turned off is so desired.

ZOOMING / TIME SCALE

The time axis can be either stretched out (in order to view more details of the chart), or condensed in order to manage to fit the chart in a smaller visible region. The three factors that determine how much of the chart will be visible in a given window space are:

1. The Viewing Mode
2. The Time Scale Chosen for Minor & Major Increments, &
3. Zooming Factor

There are two viewing modes: **Fit-to-Window** and **Nominal**. When the graph viewing mode is set to 'Fit-to-Window', the application will display the graph's contents always in the available window width. In this mode, a user can gain an overall perspective of the entire graph, at the expense of viewing small details. In this mode, it is possible that not all of the major and/or minor increments of time can be individually visible. Sometimes, the increments will be melded into two, or three or more at a time, in order for the labels to fit and in order for the entire time span to fit in the available space. In this mode priority is given to displaying the entire graph within the allotted space. In the 'Nominal' viewing mode, the application decides the scale by which to display the occupancy information in a way that the user's selection for minor increments is obeyed. In other words, in this mode, all the minor increments are displayed, more then likely requiring more horizontal space that what is available in a single window width, so a horizontal scroll is now visible. In that mode, you can further increase or decrease the zooming factor by using the **Zoom to** or **Zoom by** options of the toolbar. The **Zoom to** option will pick a zoom factor such that the chart's window will display exactly the selected span of time (a day, a month, etc.). The **Zoom by** option simply increases or decreases the zooming ratio by the selected percentage, thereby allowing more or less detailed to be visible on the graph. You can also zoom in and out by selecting the corresponding commands in the chart's command menu.

The zoom in/out and zoom to/by commands and/or buttons on the toolbar are only active if the viewing mode is set to nominal. When viewing the chart in the fit-to-window mode, the scale is automatically picked to make sure that the chart fits in the available space.

EXPORTING CHART'S DATA

The chart's scheduling, occupancy or consumption data can also be exported in a tabular format that can be readily imported into MS-Excel for further processing / plotting etc. You can select **Export Data to Excel** from the chart's command menu and then dictate a file name and location, and SuperPro Designer will include the data into the selected file.

COPYING / EXPORTING CHART AS PICTURE

You can copy the chart (as a picture) by selecting **Copy ▸ Chart** or **Copy ▸ Legend** (the latter only available in multi-batch charts). After you have issued either of the above commands, you can go to another application (e.g. MS-Word, or MS-Excel) and issue a paste

command. This will paste the chart (or the legend) as a picture in the destination document. Another way of exporting the chart (as a picture) is to save it in a Windows Metafile format ('wmf') as a file and later import the picture file into another application (like MS-Word). You can export the chart picture in Windows Metafile Format by selecting **Export Chart as Metafile** from the chart's command menu.

PRINT/PRINT PREVIEW

You can print (or print preview) a chart directly from SuperPro Designer by selecting the **Print** (or **Print Preview)** command from the chart's command menu. If the printing arrangement is not adequate, or more printing options are desired (e.g. smarter scaling, etc.) then it is recommended that you export the chart as a picture into another application first (e.g. MS-Excel) and then print it.

6.2b Equipment Gantt Chart

This chart, and for a single batch (Equipment Gantt Chart (Single Batch)), can be viewed by selecting **Tasks ▸ Gantt Charts ▸ Equipment GC**; to view the chart for multiple batches Equipment Gantt Chart (Multiple Batches), select **Tasks ▸ Gantt Charts ▸ Equipment GC (Multiple Batches)** from the main menu.

The equipment Gantt chart presents the same information on occupancy as the equipment occupancy chart, only each occupancy bar (aka task bar) in the Gantt chart can be expanded in its component activities (subtasks) where each subtask is displayed in a separate line (similar to the operations gantt chart). This makes it much easier to view any conflicts that may exist between operations and/or between procedures hosted by the same equipment. Also, subtasks may be collapsed and abstracted to aggregate activities to gain a better overview of how the process utilizes the equipment.

There are seven levels of activities considered by the equipment gantt chart. Those levels in order of hierarchy are as follows:

1. Batch
2. Branch
3. Section
4. Equipment
5. Procedure
6. Cycle
7. Operation

Each task (activity) bar in the above hierarchy expands into subtasks of the level below. Since branches and sections may not be used often in a process they can be optionally skipped and thereby have batch bars expand directly into equipment bars. This is done through the Equipment Gantt Chart Style Dialog: Contents tab. Each bar has its own visual style that can be customized by the user. It is also convenient to display next to each task bar a short description of the activity represented by the bar. You can turn on or off the textual description (perhaps only for certain types of activities, e.g. operations only) by modifying each activity's style.

The gantt chart presents a dual view of the activities/occupancy of each equipment: the graph view (on the right) and the spreadsheet view (on the left). The spreadsheet view presents (in a

column format) more pieces of information for each activity such as the start time, end time, duration, short description of the activity etc. If you right-click on a task bar you will be presented with a menu that allows you to view (and edit) the properties of the activity behind the task bar (operation, procedure, equipment, etc.) as well as its visual appearance (style). You can fully customize the contents of the spreadsheet view (on the left) as well as the appearance of the chart (on the right) by selecting **Style / Chart & Grid**.

For information on how the number of batches is calculated (for multi-batch charts), the time line settings and all the basic functionality of the chart (zooming in/out, printing, copying chart's data, copying chart as a picture, etc.), see 6.2a Equipment Occupancy Chart.

6.2c Equipment Utilization Breakdown

When multiple procedures share the same equipment resource, or when looking for opportunities for procedures to share equipment (in order to save capital) you may find viewing the utilization of each equipment in the process very helpful. This table presents the busy time of each equipment resource as how each of the hosted procedures contribute to the total busy time. You can view the Main Equipment Utilization Breakdown table by selecting **View ▸ Utilization Breakdown ▸ Main Equipment** from the main menu of the application.

6.2d Equipment Occupancy Data Table

If you would like to see all the occupancy indices (busy time, idle time, waiting time etc.) tabulated for all the equipment resources in a process then select **View ▸ Main Equipment Occupancy Data ▸ Table** from the main menu of the application. This will bring up the Main Equipment Occupancy Data Table. You can customize the contents of the table to suit your preferences. For an accurate description on the meaning of each index and how it is calculated, see 'Occupancy Indices' on page 6-17.

6.2e Equipment Occupancy Data Chart

The same occupancy indices that are presented in the equipment occupancy data table, can also be viewed in chart format. To show the occupancy data of all equipment resources in a process as a chart, select **View ▸ Main Equipment Occupancy Data ▸ Chart** from the main menu of the application. This will bring up the Main Equipment Occupancy Data Chart. You can customize the contents of the chart to suit your preferences. For an accurate description on the meaning of each index and how it is calculated, see 'Occupancy Indices' on page 6-17.

6.3 AUXILIARY EQUIPMENT

Besides the main equipment that are assumed to be hosting all unit procedures in a process, there may be other equipment that provide support in order to execute certain operations. For example, a Clean-in-Place operation requires the use of a CIP skid which engages for the entire duration of the operation. Oftentimes, the availability of such skids may be a critical issue in the planning and scheduling of a process. Another example of a supporting (auxiliary) hardware may be the presence of a transfer line that engages every time material needs to be moved from one location (equipment) to another. Once again, there may be a limited number of available transfer lines and therefore the timing of operations that need to engage them may

need to be adjusted appropriately such that there are no conflicts (overlapping use) of such facilities. SuperPro Designer currently allows the user to represent CIP (or SIP) skids and associate them with specific cleanup operations. Transfer lines and Chromatography Column Skids are not currently supported but will become available soon. Figure 6.2 shows how to activate the presence of a CIP skid during a CIP operation:

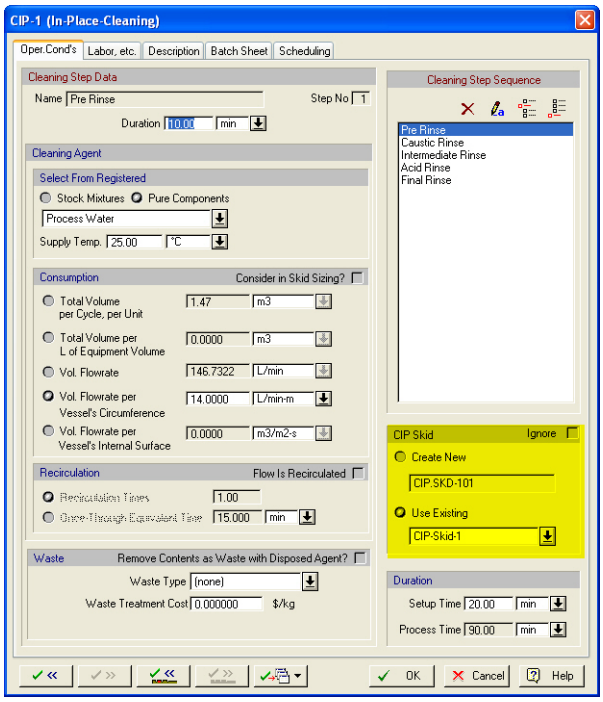


Figure 6.2: Requesting the presence of a CIP skid during a CIP operation.

Make sure the "Ignore" button above is un-checked. Then either allow a new CIP skid to be introduced (and engaged) or this operation, or click on "Use Existing" and select a name of a skid that had previously been introduced (as part of some other CIP operation). Either way, SuperPro Designer will now assume the presence of a CIP skid and will keep track of its usage.

CIP Skids, SIP Panels (essentially all auxiliary equipment) do not have a visual presence on the flowsheet of a process. The only way to view their presence is by either present a utilization table (select ***View ▸ Utilization Breakdown ▸ CIP Skids & SIP Panels*** *from the application's main menu) or by viewing the 'AuxEq' tab of the Process Explorer Toolbar.*

Since all auxiliary equipment do not have a direct visual user interface on the process flowsheet, you cannot rename or delete them directly. If you delete all the operations that utilize a specific CIP skid then the skid itself will cease to exist. SuperPro Designer will indirectly delete the skid form the list of the auxiliary equipment used by the process. The same will happen if you visit all operations that utilize a specific skid and request that they not use a

CIP skid. In that case, the application will again remove the CIP skid from the list of utilized auxiliary equipment.

If you wish to no longer engage a specific CIP skid in any CIP operation without deleting the operations themselves (essentially delete a CIP skid from the list of auxiliary equipment used by the process) then instead of visiting all the CIP operations i/o simulation dialogs and disengage the skid one-at-a-time, visit the 'AuxEq' tab of the Process Explorer, select the skid that you wish to delete and then select the **Delete** *button ( ).*

If you wish to rename an existing skid, it can only be done from the Process Explorer. Visit the 'AuxEq' tab of the Process Explorer, then select the skid you wish to rename and click on the **Rename** button ( ).

The property data of auxiliary equipment can be also inspected from the Process Explorer Toolbar (Aux. Equipment tab) by clicking on the **View/Edit** button ( ). This brings up the Auxiliary Equipment Properties Dialog.

SIZING

Whenever an auxiliary equipment is engaged in a related operation, a user may choose to activate an option on the operation that dictates to the application to consider the demands of that particular operation on the sizing of any related equipment. For example, consider CIP skids and CIP operations. A CIP operation can be made up from several cleaning steps strung together. For each step, you can check a choice ("Consider in Sizing") on its 'Oper.Conds' tab. If this choice is set, then the size of the CIP skid's tank will be adjusted so that it can hold the amount of material required for that cleaning step. Of course, if the same skid is engaged in several steps (and/or several CIP operations) the final size of the skid's tank will be determined by the largest demand on cleaning material volume. The size of the auxiliary equipment is presented in the process explorer view of all auxiliary equipment ('AuxEq' tab) as well as in the equipment report. The demands of each sizing operation are also shown in the auxiliary equipment utilization breakdown table, see 6.4d Auxiliary Equipment Utilization Breakdown.

OCCUPANCY INDICES

Just as used in the context of main equipment utilization, **busy time** for an auxiliary equipment represents the total amount of time (during the span of a recipe cycle time) that the equipment is presumed as 'engaged' by some operation. And just like main equipment, the **busy time fraction** (or percentage) is the ratio of an auxiliary equipment's busy time over the process cycle time. Note that unlike main equipment resources, we allow auxiliary equipment to be used by operations of follow-up batches even before all operations of the current batch are not done using it. In other words, we don't block the time between operation engagements of the same batch. The complementary measure to the busy time, is the **idle time**. This is the time (during cycle time) that the auxiliary equipment is not engaged by any operation. And the **idle time fraction** (or percent) is the ratio between the idle time and the recipe cycle time.

Given the shortage of auxiliary equipment, it is important that they are utilized most efficiently and in a balanced way. SuperPro Designer calculates two indices that help you gauge how well your auxiliary equipment are being engaged by the process:

Relative Load (RL): The ratio between the busy time of an auxiliary equipment over the total busy time of all equipment (of the same nature). Assuming that all skids are interchangeable, you don't want to have some skids have a RL factor close to 100% while others are below 50%.

Relative Utilization (RU): The ratio between is the busy time of an auxiliary equipment to the process batch time. It is similar to the busy time fraction, only the RU fraction is with respect to the process batch time as opposed to the recipe's cycle time.

All of the above factors are presented in the process explorer view of all auxiliary equipment ('AuxEq' tab). Furthermore, the occupancy indices as well as a detailed breakdown to all contributing operations can be seen in the auxiliary equipment utilization breakdown table, see 6.4d Auxiliary Equipment Utilization Breakdown.

6.4 AUXILIARY EQUIPMENT CHARTS & TABLES

Occupancy information for auxiliary equipment can be just as important as main equipment's, especially in processes currently in operation where the number of available auxiliary equipment to fit the needs of this process may be limited. SuperPro Designer presents a utilization information on the currently supported auxiliary equipment (CIP Skids and SIP Panels) in a variety of formats (similar to main equipment).

6.4a Auxiliary Equipment Occupancy Chart

This chart is essentially part of the main equipment occupancy chart (EOC) assuming auxiliary equipment are allowed to be presented. The Equipment Occupancy Chart (Single Batch) and Equipment Occupancy Chart (Multiple Batches) are presented when you select **Single Batch** or **Multiple Batches**, respectively, on the **Charts ▸ Equipment Occupancy** menu of the application. By default, the EOC for a process will include on the y-axis all main equipment as well any auxiliary equipment (CIP Skids, SIP Panels) currently utilized by the process. However, selecting **Include / Exclude / Order Equipment** from the right-click menu of the chart allows you include exclusively (if needed) just the auxiliary equipment of your choice in the chart. The same command is also available from the Equipment Occupancy Chart Style: Contents Tab.

For a full description of all services offered by the equipment occupancy chart, see 6.2a Equipment Occupancy Chart.

6.4b Auxiliary Equipment Gantt Chart

The auxiliary equipment gantt chart is shared with the main equipment gantt chart (EGC). The Equipment Gantt Chart (Single Batch) and Equipment Gantt Chart (Multiple Batches) are presented when you select **Equipment GC** or **Equipment GC (Multiple Batches)**, respectively, on the **Tasks ▸ Gantt Charts** menu of the application. You can customize the contents of the main equipment's gantt chart to show both main and auxiliary equipment or just auxiliary equipment. By default, the EGC for a process will include all main equipment as well any auxiliary equipment (CIP Skids, SIP Panels) currently utilized by the process. However, selecting **Include / Exclude / Order Equipment** from the right-click menu of the chart allows you include exclusively (if needed) just the auxiliary equipment of your choice in the chart. The same command is also available from the Equipment Occupancy Chart Style: Contents Tab.

For a full description of the equipment Gantt chart, see 6.2b Equipment Gantt Chart.

6.4c Auxiliary Equipment Demand

As auxiliary equipment (like CIP skids) are sometimes a bottleneck in the scheduling of a process, users may find the auxiliary equipment demand chart very useful in answering the following question: "Given the current scheduling of operations in my process, how many skids are needed to service the CIP operations?" Note that in answering the question we don't have to set specific assignments of skids to operations. This chart essentially tracks how many CIP operations (that require a skid) are 'on' (or active) during the execution of a single batch or during multiple (stacked) batches. The CIP Skid demand Chart (Single Batch) and CIP Skid demand Chart (Multiple Batches) are presented when you select **Single Batch** or **Multiple Batches**, respectively, on the **Charts ▸ Aux. Equipment Demand ▸ CIP Skids** menu of the application. Similarly, the SIP Panels demand Chart (Single Batch) and SIP Panel demand Chart (Multiple Batches) are presented when you select **Single Batch** or **Multiple Batches**, respectively, on the **Charts ▸ Aux. Equipment Demand ▸ SIP Panels** menu of the application.

6.4d Auxiliary Equipment Utilization Breakdown

Once specific assignments of auxiliary equipment to operations that require them have been made, users need to know how 'heavy' is the current utilization of available units. Such information can be used in two ways:

(a) Realign the engagements such that there is a more evenly distributed use of the equipment

(b) If there is a need for a new assignment, use the equipment that is currently less utilized

The auxiliary equipment utilization breakdown can be presented when you select **View ▸ Utilization Breakdown ▸ Aux. Equipment** the from the main menu of the application. For a detailed definition of all the terms that appear in the table (busy time/fraction, idle time/fraction, relative load (RL) and relative utilization (RL), see 'Occupancy Indices' on page 6-17.

6.5 MATERIALS

The term 'materials' as used in SuperPro Designer covers all substances that appear anywhere and for any purpose in the process. There are two types of substances that can be introduced (registered) in a process: pure components and stock mixtures (or mixtures for short). To register a new pure component please choose **Tasks ▸ Pure Components ▸ Register, Edit/View Properties** from the main menu of the application. To register a new mixture please chose **Tasks ▸ Stock Mixtures ▸ Register, Edit/View Properties**. For details on how to register new components and mixtures, see 3.1a Pure Component Registration and 3.2a Stock Mixture Registration. Materials become available to operations by means of:

(a) Streams (attached to the input port of the procedure),

(b) Equipment contents (initialized at the beginning of a batch), or

(c) User selection on the i/o simulation dialog of an operation

An example of case (c) above is when selecting a specific cleaning agent for a CIP operation or a sweeping agent as part of a gas sweep operation. Note that in this case, the selected material becomes available to the operation but does not appear on a procedure input stream.

Material that becomes available to an operation though its i/o simulation dialog may either join the rest of the material already present in the equipment contents (e.g. pressurize operation) or leave the equipment through one of the procedure's output streams (e.g. gas sweep operation's emission stream) or leave the equipment without the presence of a stream (e.g. CIP operation's wash/waste stream). There is even the rare case of the sampling operation that allows a (small) amount of material already present in the (liquid) equipment contents to leave the process without a stream. In summary, materials leave the process by means of:

(a) Streams (attached to output streams of the procedure)

(b) Equipment contents (or equipment's local receptacle), or

(c) User's choice on operation's dialog (e.g. sampling and CIP operation) and without being present on an output stream.

6.5a Entering Material Consumption Classification

Regardless of how material makes itself available to the process for consumption (input stream, equipment contents or i/o simulation dialog choice), SuperPro Designer distinguishes the following five categories as possible consumption origins (aka consumption classification):

1. Raw Material
2. Cleaning Agent
3. Heat Transfer Agent
4. As part of a Revenue Stream
5. As part of an Unclassified Stream

If the material enters the process via an input stream, then its consumption classification follows the stream's classification. Typically an input stream will be automatically classified as 'Raw Material' and therefore all consumption of material carried by the stream will also be tallied under the 'Raw Material' origin. If a user changes the classification of an input stream to 'Cleaning Agent', 'Revenue' or 'Unclassified', then any material carried on that input stream will be tallied under the corresponding category. Material that participates in the process as part of the initial contents of equipment, it is always assumed as 'Raw Material' but its cost may or may not be taken into account (as part of the operating cost). Finally, material that enters the process without a stream, is automatically classified based on its intended use and cannot be changed by the user. For the cases of pressurize and gas sweep, the material is classified as 'Raw Material'; the case of CIP operation, the material is classified as 'Cleaning Agent'.

A word needs to be mentioned here for the 'Heat Transfer Agent' category. If the user has chosen to associate a specific material to any of the heat transfer agents registered in the process (see 6.7 Heat Transfer Agents), then any time that heat transfer agent is employed by an operation, the equivalent amount of material (as dictated by the agent's definition) is assumed that is 'consumed' as 'Heat Transfer Agent' material. Please note that this is not an accurate representation as this material is presumed to be needed at the time that the heat transfer agent is generated by the utility service system, not when it is consumed. If users are using this feature, they are advised to ignore the 'Heat Transfer Agent' as origin from the consumption

charts. Of course the consumption of heat transfer agent related material will add to the operating cost of the process.

6.5b Exiting Material Classification

Since most material will leave the process on an output stream, the classification of the exiting material follows that of the output stream. Therefore we consider the following seven categories:

1. Revenue
2. Credit
3. Emission
4. Aqueous Waste
5. Organic Waste
6. Solid Waste
7. Unclassified

For the rare exception of material exiting the process without a stream the designation is provided directly on the i/o simulation dialog of the corresponding operation (sampling or CIP). If no specification is provided, then 'Unclassified' will be assumed.

Finally, material can leave the process as either final contents of equipment (not removed by the end of the batch) or left in the local receptacle (if the automatic emptying of contents feature has been activated, see 6.1e Local Receptacle & Automatic Emptying of Contents). Material left in vessels will be assumed as 'Unclassified' (and cannot be changed by the user), whereas material left in a receptacle is tagged as 'Unclassified' but can be given a user-chosen classification form the dialog that activates the automatic emptying of equipment before reuse (click **Equipment Contents ▸ Before Reuse ▸ Empty to Local Receptacle** from the procedure's command menu to display the Empty Contents Before Reuse Dialog).

Please note that even if he automatic emptying feature for an equipment resource is activated, the final contents of equipment (as left by the last procedure using the equipment) will not be removed to the local receptacle. If it is imperative that the leftover material be treated as waste (and perhaps associate some waste treatment cost to it) then, the user must make sure that the final contents are removed with a transfer out operation, and the associated output stream be tagged as appropriate waste with an appropriate waste treatment cost.

6.5c Material Rates and Timing

For every material that enters (or exits) the process the application associates an event (operation) that is responsible for the transfer. The rate of material transfer is either set (or calculated) directly from the associated operation (e.g. the charge rate or CIP cleaning rate) or the total amount is set (or calculated) by the operation and then a rate is calculate by dividing the total amount with the process time of the operation. In other words, we always assume that the material flows in (or out) evenly during the process time of an operation.

Material that is found at the beginning of the batch as equipment contents it is not considered as 'entering' the process and therefore it is not associated with any operation. Similarly, material found at the end of the process as final equipment contents it is not considered as 'exiting' the process and it is similarly not associated with any operation. Neither amount will appear on the material consumption or production charts.

There are two special cases that need to be mentioned. When material enters a procedure via the auto-initialize feature (see 5.5a Default Input Ports & Auto-Initialization), then the material's rate and timing will be associated with the first operation in the procedure's queue, even though, clearly that operation may not be responsible for bringing the material into the procedure. Similarly, when material leaves the a unit procedure via the auto-removal feature (see 5.5b Default Output Port & Auto-Removal) then its timing will be associated with the operation last in the queue. For material removed from equipment before reuse via the auto-emptying feature (and placed to the local receptacle, see 6.1e Local Receptacle & Automatic Emptying of Contents) once again, the last operation in the procedure's queue will be used. If the timing for the above material transfers is of importance, then the user is urged to employ a transfer in (or charge) and/or a transfer out in order to better capture the timing of the material transfer.

Detailed charts for material entering or exiting a process can be generated for any material present (registered) in the process (see **Charts ▸ Material ▸ Entering** or, **Charts ▸ Material ▸ Exiting** under the main menu of the application).

6.5d Material Inventory

Besides keeping track of material consumption, it is possible to provide the application with enough information about the replenishing process (for a given material) so that it can present you with a detailed material inventory chart. For example, if you specify the holding capacity of the storage for that material as well as the rates and frequency of supply, then the application can provide you with a inventory chart for the entire supply, demand and accumulation information. Similarly for material leaving the process, besides viewing material output charts, users can provide the application with storage capacity and removal rate and frequency information and the application will present a detailed inventory chart for a given material.The inventory information for entering materials can be accessed from the **Tasks ▸ Other Resources▸ Materials, Entering** interface. Select the material and click on the **View/Edit** button ( ) (or double-click the material's row) and you will be presented with the Entering or Exiting Material Properties Dialog with information regarding the (entering) material as resource. The 'Inventory Data' tab allows you to view and edit inventory information (on the supply side) for this material. The same information for the material as a resource exiting the process, can be viewed from the **Tasks ▸ Other Resources▸ Materials, Exiting** interface. The inventory charts can be accessed from the **Charts ▸ Material ▸ Entering, Inventory** or, **Charts ▸ Material ▸ Exiting, Inventory** under the main menu of the application.

6.5e Material Storage Units

Material consumption (or output) charts and material inventory charts deal with the consumption or production of a given material as it enters or exits everywhere in the process. Even though the classification of the material can be narrowed down (e.g. track only 'Raw Material' entering the process, or track only 'Aqueous Waste' leaving the process) these charts cannot be customized to localize the source for the consumption or production of material. For users who want to refine the tracing of material consumption and/or production based on its consuming (or producing) location in the process, SuperPro Designer offers as solution the concept of 'Storage Units'. You can define a supply storage unit and hook it up to service only certain parts of a process where, say, WFI is used. Later, you can ask to see consumption and/or inventory charts for that storage unit alone, and therefore be able to track the use of WFI for

only those points of consumption that you chose. For more details on how to introduce storage units and use them in your process, see 6.13 Material Storage Units.

6.6 MATERIAL CHARTS & TABLES

6.6a Material Consumption & Material Output Charts

You can view in a chart the detailed rate of consumption for a given material by selecting **Charts ▸ Material ▸ Entering ▸ Single Batch** (Entering Material Consumption Chart (Single Batch)) or **Charts ▸ Material ▸ Entering ▸ Multiple Batches** (Entering Material Consumption Chart (Multiple Batches)) from the main menu of the application. In a continuous process that contains batch procedures the same chart can be displayed by selecting **Charts ▸ Material ▸ Entering ▸ Selected Time Horizon** from the main menu. Before the chart is presented, you will be prompted to choose:

1. A material amongst all registered ingredients (pure components or mixtures), and
2. The consumption origins that you wish to be included when collecting consumption rates (see 6.5a Entering Material Consumption Classification).

Besides the actual consumption rate curve, users can chose to see at on the same chart the following lines:

1. A time-averaged consumption rate line (averaged over a user-specified periodic window); for example, users may be interested in seeing the consumption rate of a given buffer in 8-hour average values. Such lines can provide insight in designing the production rate of the replenishing process.
2. A cumulative amount line: Amount total may be of interest when considering inventory capacity. Users may also specify a time period after which the accumulated amount gets reset to 0.0.

The style of the consumption chart dictates exactly which lines will be plotted. As part of the chart's style you can also specify the rate units and the amount units to be used for the chart, as well as the visual characteristics of the lines (color, thickness, etc.) The time-line parameters used (absolute vs relative time scale, minor/major intervals & gridmarks, etc.) are, by default, those kept by the process document. They can, of course, be customized for the consumption charts if needed. The chart's style can be changed through the Material Chart Style Dialog.

The unit choices for plotting rates and cumulative amounts are 'remembered' by the application in association with the material being plotted. In other words, you can specify a set of units to be used when viewing material-A (e.g. kg/h for rate and kg for amounts) and a different set of units to be used when viewing material-B (e.g MT/day and MT). On the other hand, the rest of the properties of the graph style (line characteristics, time line properties, etc.) will be used for all material charts (regardless of the material chosen).

DEFAULT NUMBER OF BATCHES

See 'Default Number of Batches' on page 6-12.

TIME LINE

See 'Time Line' on page 6-12.

ZOOMING / TIME SCALE

See 'Zooming / Time Scale' on page 6-13.

EXPORTING CHART'S DATA

See 'Exporting Chart's Data' on page 6-13.

EXACT VS DISCRETIZED CONSUMPTION DATA

If you are exporting consumption and/or inventory data, before you select the destination file for the data, you may also want to chose to discretize the data to an interval of your choice. One of the most common reasons for exporting consumption data is to combine data from different processes in order to view the cumulative effect on a central utility server (e.g. for high pressure steam). If you do not discretize the data, then each process will export values that will be changing at different time steps making it very difficult to combine them. On the other hand, choosing a common discretization interval, will provide a common platform for all the exported processes and making the addition of the data very easy. The choice of exporting exact vs discretized data is done in the Export Resource Tracking Data to Excel Dialog.

COPYING / EXPORTING CHART AS PICTURE

See 'Copying / Exporting Chart As Picture' on page 6-13.

PRINT / PRINT PREVIEW

See 'Print/Print Preview' on page 6-14.

The counterparts of entering (consumption) charts are the exiting (output) charts. Such charts are of particular importance when tracking waste and waste amounts (e.g. emissions). The output charts can be generated by selecting **Charts ▸ Material ▸ Exiting ▸ Single Batch** (Exiting Material Output Chart (Single Batch)) or **Charts ▸ Material ▸ Exiting ▸ Multiple Batches** (Exiting Material Output Chart (Multiple Batches)) or **Charts ▸ Material ▸ Exiting ▸ Selected Time Horizon** from the main menu of the application. Before the chart is presented you will be prompted to choose:

1. A material amongst all registered pure components, and
2. The material output classification that you wish to be included when collecting output rates, see 6.5b Exiting Material Classification.

When generating an output chart, the list of choices for ingredient includes pure components only. Stock mixtures do not have a presence anywhere other than at the input locations for a process (input streams, equipment contents, agents selected directly for an operation).

Just as in the case of consumption charts, besides the rate curve, you can choose to include a time-average rate curve and/or a curve tracking the cumulative amount produced. The settings for which lines included in the chart along with visual choices for the lines as well the time-line characteristics are all part of the style of the chart (Material Chart Style Dialog).

6.6b Material Consumption Inventory & Material Output Inventory Charts

When considering the consumption of a material, it is often of importance to design inventory capacity and/or select a preferred replenishing rate so that the process never runs out of material and at the same time, excessive amounts of storage are avoided. SuperPro Designer will not design the inventory system for you automatically. The time-averaged consumption rate curve and time-reset cumulative curve presented on the consumption chart provide good clues on what should be your targets for replenishing rate and storage capacity correspondingly, see 6.6a Material Consumption & Material Output Charts. However, it is up to the user to provide the application with a suggested inventory strategy then the application can generate an inventory chart that will show material amounts in the holding tank during one or several overlapping batches. The following inventory information needs to be specified before an inventory chart is generated:

1. Storage capacity
2. Initial contents
3. Lower & upper limits on storage capacity (if anything other than 0% and 100%)
4. Supply (replenishing) rate
5. Supply (Replenishing) policy: Need a start time when policy activates and an on/off triggering mechanism (either tied to inventory level or tied to a regularly timed schedule).

Inventory parameters are specified through the Entering or Exiting Material Dialog: Inventory Data tab.

You can view inventory charts by selecting **Charts ▸ Material ▸ Entering, Inventory ▸ Single Batch** (Entering Material Inventory Chart (Single Batch)) or **Charts ▸ Material ▸ Entering, Inventory ▸ Multiple Batches** (Entering Material Inventory Chart (Multiple Batches)) from the application's main menu. In a continuous process that contains batch procedures the same chart can be displayed by selecting **Charts ▸ Material ▸ Entering, Inventory ▸ Selected Time Horizon** from the main menu.

For the basic common services offered by all time charts (setting the number of batches, zooming in/out, adjusting the time scale, copying the chart as picture, copying chart data to Excel, printing, etc.), see 6.6a Material Consumption & Material Output Charts.

Similar inventory charts can be generated on the output side of the process, by selecting **Charts ▸ Material ▸ Exiting, Inventory ▸ Single Batch** (Exiting Material Inventory Chart (Single Batch)) or **Charts ▸ Material ▸ Exiting, Inventory ▸ Multiple Batches** (Entering Material Inventory Chart (Multiple Batches)) or **Charts ▸ Material ▸ Exiting, Inventory ▸ Selected Time Horizon** from the application's main menu. This time, besides selecting a pure component, the user must also provide a holding capacity and a removal strategy (essentially the same items of information as for the supply inventory above, items 1 through 5).

6.6c Material Consumption (Demand) Tables

The process keeps a detailed log of all materials present. If you wish to have a direct view of all the materials present currently, you can open the process explorer and pick the 'Matl' tab of the Process Explorer Toolbar. This tab will present a quick reminder of all the pure components and/or stock mixtures registered.

If you are interested in seeing the total demand for materials then you should visit the List of Entering Materials (& View of Total Consumption Demand) dialog shown when you select **Resources ▸ Materials, Entering** from the flowsheet's context (right-click) menu or **Tasks ▸ Other Resources ▸ Materials, Entering** from the application's menu. This dialog will itemize all materials currently registered in the process, their total demand (per batch or per year), their price and total cost. The totals presented can be customized to include contributions from only some origins (e.g. 'Raw Materials' only).

If you are interested in tracking down the locations and rates where a given material is being consumed, then select **Resource Demand Breakdown ▸ Materials** from the application's main menu. This will bring up the Entering Material Demand Breakdown dialog that presents in a tree-like view (with top nodes each material) the demand for each material and how all the exact sources where they are needed. Once again, the presented amounts can be customized to only aggregate material from certain origin(s) and they can include / exclude only the materials of your choice.

6.6d Material Production (Output) Table

In order to view total outputs for materials exiting the process, select **Resources ▸ Materials, Exiting** from the flowsheet's context (right-click) menu or **Tasks ▸ Other Resources ▸ Materials, Exiting** from the application's menu. This will bring up the Entering or Exiting Material Properties Dialog that presents in a list all materials currently registered in the process, their total output (per batch or per year) and their selling price or waste treatment cost. The totals presented can be customized to include contributions from only some origins (e.g. 'Raw Materials' only).

If you are interested in tracking down the locations where a given material is being consumed, then select **Resource Demand Breakdown ▸ Materials** from the application's main menu. This will bring up the Entering Material Demand Breakdown dialog that presents in a tree-like view (with top nodes each material) the demand for each material and how all the exact sources where they are needed. Once again, the presented amounts can be customized to only aggregate material from certain origin(s) and they can include / exclude only the materials of your choice.

6.7 HEAT TRANSFER AGENTS

A heat transfer agent is an agent used to carry out a heating or cooling task as required by the performance of the unit procedure. Demand for heat transfer agents is calculated by operations that perform heating or cooling. SuperPro Designer keeps track of the instantaneous as well as cumulative demand of heat transfer agents.

Auxiliary utilities can also be specified for each operation to account for any cooling or heating consumption that is not currently computed by the simulation model. You can set the auxiliary utilities for an operation through the Operations Dialog: Labor, etc Tab. When auxiliary heating and cooling are specified, the provided values are not used in heat balances. They are only used in calculating the total utility consumption and the operating cost of that operation (and the associated equipment).

ENERGY RECOVERY

The demand for heat transfer agents may be reduced by recovering the excess energy from hot operations and matching it with cold operations which require heating. For more details on recovering energy in SuperPro Designer see the Energy Recovery topic.

6.7a Definitions in the 'System' Database and in the 'User' Database

The Designer portion of the agent databank maintains a (currently limited) list of options for heat transfer agent types. To review the list of such available agents, select **Databanks ▸ Heat Transfer Agents** from the main menu (or hit **F3** as a shortcut). This will bring up the Heat Transfer Agents Databank Dialog. User-defined heat transfer agents can also be introduced in the agent databank and saved in the 'User' database. Changes made to the heat transfer agents databank do not affect existing process files or other parts of the databank even if the edited heat transfer agents are used as the basis for utilities declared in sites.

For more details on the Heat Transfer Agents Databank, please see 15.7 Heat Transfer Agents Databank.

6.7b Registered (in use) Heat Transfer Agents

When selecting a heat transfer agent for an operation, you can choose from a list of generic-type agents defined in the databanks or, for operations belonging to allocated sections (see 'Section Allocation' on page 8-6), from the corresponding site utilities. Agents currently in use can then be inspected from the List of Heat Transfer Agents Currently in Use dialog accessed by selecting **Edit ▸ Process Options ▸ Resources ▸ Heat Transfer Agents** or **Tasks ▸ Other Resources ▸ Heat Transfer Agents** from the main menu. From here you may edit the properties of a heat transfer agent. See 6.7d Heat Transfer Agent Properties.

6.7c Heat Transfer Agents in Sites

To add, edit or delete heat transfer agents declared as utilities in sites, select **Databanks ▸ Sites and Resources** from the main menu. From the Sites & Resources Databank Dialog that appears, you can select the desired site from the left pane (site tree) and the utilities node on the right pane and you may add new, edit, or delete heat transfer agents by clicking on the appropriate button from the toolbar.

When adding a new site utility you will be presented with a dialog which displays all currently available heat transfer agent definitions in the agent databank. From there you can select one or more agents that you want to include in the site.

Once a heat transfer agent is added to a site as a site utility then you cannot delete it from your agent databank; first you must remove the agent from the site and then you are free to delete the agent from your agent databank.

If a section is allocated to a site, then available to operations of this section are not only utilities of this site but of its parent sites as well. This implies that if there is a central utility plant in a site then all produced utilities are available to all sub-facilities within that site.

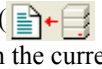
Changes made in site utilities may affect existing process files (opened or closed at the time of the modification) that contain sections that use them. SuperPro Designer will not attempt to reconcile any process files currently not open in by the program. However, SuperPro will require that any open process files be consistent with the state of currently available resource databanks. Therefore, all changes done in the site and resources databank will automatically be

propagated to open process files even if de-allocation (i.e. substitution with generic-type utilities) is needed to maintain consistency. Such changes could affect both material balances as well as economic results so re-solving M&E balances might be needed for all affected process files.

For more details, see 15.7b Adding or Deleting a Heat Transfer Agent.

6.7d Heat Transfer Agent Properties

The parameters of a heating/cooling agent as shown in the heat transfer agents databank are the default parameters that are used the first time any of the processing steps in your process file employs that heating/cooling agent. If you decide to use different values for your specific process file, then you can adjust those parameters without affecting the default values of the agent in the databank, by bringing up the List of Heat Transfer Agents Currently in Use that appears when you select the **Edit ▸ Process Options ▸ Heat Transfer Agents** option from the main menu, or just the **Resources ▸ Heat Transfer Agents** option from the flowsheet context menu. The dialog that pops up displays a list with all heat transfer agents currently employed by the process file.

To view or edit the properties of a heat transfer agent, you should click on the agent's index column to select it and then press the **View/Edit Properties** button ( ). Alternatively you can double-click on the agent's index column. The Heat Transfer Agent Properties Dialog that comes up contains the agent's data organized in three tabs. Changes made in the heat transfer agent through this dialog will only affect this process file; they will not be stored in the Heat Transfer Agents Databank. If you want the agent in this process file to take up the properties of the agent in the databank (in case they are different) select the agent by clicking on the agent's index column and press the **Update Properties from DB Record** button (). If you want to update the databank's record (heat transfer agent properties) based on the current process file's record press on the **Deposit/Update Record in DB** button ( ).

The **Properties** tab lets you define the type of the agent (heating or cooling), the temperature at which the agent is available from the utilities support plant and the temperature at which it should be returned to the utilities plant and the cost charged for the use of this agent in $/1000 kg. Note that only through the databank you can change the type of an agent and, as mentioned before, even if you do that, that change will not affect process files that make use of this agent.

The **Availability Limits** tab lets you define bounds on consumption of this agent. There are two types of limits: rate limits (instantaneous or time-averaged over a user-defined time span) and cumulative limits over a user-defined time span. Upon request, these limits will be plotted on the resource consumption charts (see 6.8a Heat Transfer Agent Consumption Chart) so that you can compare them against the actual consumption.

The **Inventory Data** tab lets you define storage and supply data for this agent that, in turn, will be used to calculate the inventory chart lines (see 6.8b Heat Transfer Agent Consumption Inventory Chart). This tab is displayed only when the heat transfer agent has been defined to be storable. This is done by editing the corresponding check box in the Heat Transfer Agents Properties tab. No inventory charts can be created for non-storable agents.

Note that, for site utilities, data in the Properties and Availability Limits Tab are not editable through the Heat Transfer Agents Currently in Use dialog. The reason is that site utilities could

be shared by different process files and only through the site databanks their properties can be modified. To edit those values, you will need to visit the sites databank through the **Databanks ▸ Sites & Resources** menu item as explained before.

The locations where a heat transfer agent is currently utilized in the process can be viewed by clicking on the button . This can be in operations, which are displayed in order of first use accompanied with their hosting procedure.

6.8 HEAT TRANSFER AGENT CHARTS & TABLES

6.8a Heat Transfer Agent Consumption Chart

You can view in a chart the detailed rate of consumption for a given heat transfer agent by selecting **Charts ▸ Heat Transfer Agent ▸ Consumption ▸ Single Batch** (Heat Transfer Agent Demand Chart (Single Batch)) or **Charts ▸ Heat Transfer Agent ▸ Consumption ▸ Multiple Batches** (Heat Transfer Agent Demand Chart (Multiple Batches)) from the main menu of the application. In a continuous process that contains batch procedures the same chart can be displayed by selecting **Charts ▸ Heat Transfer Agent ▸ Consumption ▸ Selected Time Horizon** from the main menu. Before the chart is presented, you will be prompted to choose whether you wish to plot a heating or cooling agent and the agent from the list of used agents.

Besides the actual consumption rate curve, users can chose to see at on the same chart the following lines:

1. A time-averaged consumption rate line (averaged over a user-specified periodic window); for example, users may be interested in seeing the consumption rate of a given buffer in 8-hour average values. Such lines can provide insight in designing the production rate of the replenishing process.
2. A cumulative amount line: Amount total may be of interest when considering inventory capacity. Users may also specify a time period after which the accumulated amount gets reset to 0.0.

The style of the consumption chart dictates exactly which lines will be plotted. As part of the chart's style you can also specify the rate units and the amount units to be used for the chart, as well as the visual characteristics of the lines (color, thickness, etc.) The time-line parameters used (absolute vs relative time scale, minor/major intervals & gridmarks, etc.) are, by default, those kept by the process document. They can, of course, be customized for the consumption charts if needed. The chart's style can be changed through the Utility Chart Style Dialog.

The unit choices for plotting rates and cumulative amounts are 'remembered' by the application in association with the utility being plotted. In other words, you can specify a set of units to be used when viewing utility-A (e.g. kg/h for rate and kg for amounts) and a different set of units to be used when viewing utility-B (e.g MT/day and MT). On the other hand, the rest of the properties of the graph style (line characteristics, time line properties, etc.) will be used for all utility charts (regardless of the utility chosen).

For the basic common services offered by all time charts (setting the number of batches, zooming in/out, adjusting the time scale, copying the chart as picture, copying chart data to Excel, printing, etc.), see 6.6a Material Consumption & Material Output Charts.

6.8b Heat Transfer Agent Consumption Inventory Chart

When considering the consumption of a heat transfer agent, it is often of importance to design inventory capacity and/or select a preferred replenishing rate so that the process never runs out of an agent and at the same time, excessive amounts of storage are avoided. SuperPro Designer will not design the inventory system for you automatically. The time-averaged consumption rate curve and time-reset cumulative curve presented on the consumption chart provide good clues on what should be your targets for replenishing rate and storage capacity correspondingly, see 6.8a Heat Transfer Agent Consumption Chart. However, it is up to the user to provide the application with a suggested inventory strategy then the application can generate an inventory chart that will show utility amounts in the holding tank during one or several overlapping batches. Before any inventory information for a heat transfer agent can be specified first you must define that the agent is storable. This is done by editing the corresponding check box in the Heat Transfer Agents Properties tab (see 6.7d Heat Transfer Agent Properties). The inventory information needed in order to generate an inventory chart is the following:

1. Storage capacity
2. Initial contents
3. Lower & upper limits on storage capacity (if anything other than 0% and 100%)
4. Supply (replenishing) rate
5. Supply (Replenishing) policy: Need a start time when policy activates and an on/off triggering mechanism (either tied to inventory level or tied to a regularly timed schedule).

Inventory parameters can be specified through the Heat Transfer Agent Properties Dialog: Inventory Data tab.

You can view inventory charts by selecting **Charts ▸ Heat Transfer Agent ▸ Inventory ▸ Single Batch** (Heat Transfer Agent Inventory Chart (Single Batch)) or **Charts ▸ Heat Transfer Agent ▸ Inventory ▸ Multiple Batches** (Heat Transfer Agent Inventory Chart (Multiple Batches)) or **Charts ▸ Heat Transfer Agent ▸ Inventory ▸ Selected Time Horizon** from the application's main menu.

For the basic common services offered by all time charts (setting the number of batches, zooming in/out, adjusting the time scale, copying the chart as picture, copying chart data to Excel, printing, etc.), see 6.6a Material Consumption & Material Output Charts.

6.8c Heat Transfer Agent Consumption (Demand) Table

The process keeps a detailed log of all heat transfer agents present. If you wish to have a direct view of all the agents present currently, you can open the process explorer and pick the 'Util' tab of the Process Explorer Toolbar. This tab will present a quick reminder of all the heat transfer agents registered in the process.

If you are interested in seeing the total demand for heat transfer agents then you should visit the List of Heat Transfer Agents Currently in Use shown when you select **Resources ▸ Heat Transfer Agents** from the flowsheet's context (right-click) menu or **Tasks ▸ Other Resources ▸ Heat Transfer Agents** from the application's menu. This dialog will itemize

all heat transfer agents currently in use in the process, their total demand (per batch or per year), their price and total cost.

If you are interested in tracking down the locations and rates where a given heat transfer agent is being consumed, then select **Resource Demand Breakdown ▸ Heat Transfer Agents** from the application's main menu. The Heat Transfer Agent Demand Breakdown dialog that appears will present in a tree-like view (with top nodes each heat transfer agent) the demand for each agent and how all the exact sources where they are needed.

6.9 POWER

Electric power requirements are defined by the user or calculated by the program for every operation that may need power to be carried out. Auxiliary power can also be specified for each operation (from the Operations Dialog: Labor, etc Tab) to account for needs not accounted for by the operations models. Additional power demand may be assigned to a section directly (from the Operating Cost Adjustments Dialog: Utilities Tab) without directly associating the consumption with any particular process step. At the section level one can define additional power consumed by unlisted equipment (skids, storage units etc) as well as power due to the general load of the plant. By default the program will use the standard power type to represent the demand in power, but the user may define his own types of power.

From version 8.0 power may also be generated from certain procedures. The procedures that are capable of producing power are the following:

- Power Generation in a Single-Stage Steam Turbine
- Power Generation in a Multi-Stage Steam Turbine
- Power Generation in a Single-Stage Gas Turbine
- Power Generation in a Multi-Stage Gas Turbine
- Steam Generation Procedure

SuperPro Designer keeps track of the instantaneous as well as cumulative demand or production of power types.

6.9a Definitions in the 'System' Database and in the 'User' Database

The 'Designer' portion of the power type databank currently contains only the standard type of power which is the power type that is also registered by default in a new process. To review the properties of the standard power type, select **Databanks ▸ Power Types** from the main menu. This will bring up the Power Types Databank Dialog. From the same interface the user may introduce new power types in the User database. Changes made in the power databank do not affect existing process files or other parts of the databank even if the edited power types are used as the basis for power declared in sites.

6.9b Power Types Currently Consumed (or Produced) by the Process

The application registers in the process file by default the standard power type for use in operations or sections. If other types of power are required, you can choose them from a list of generic power types defined in the power types databank or, for operations belonging to

allocated sections (see 'Section Allocation' on page 8-6), from the corresponding site's availale options for power types. Power types currently consumed (or produced) can then be inspected from the List of Power Types Currently Consumed by the Process or List of Power Types Currently Generated by the Process accessed by selecting **Edit ▸ Process Options ▸ Resources ▸ Power** or **Tasks ▸ Other Resources ▸ Power** from the main menu. From here you may edit the properties of a power type (see 6.9d Power Type Properties).

If the process does not contain any power generating unit procedures then you may only see the power types currently consumed. As soon as a unit procedure that can produce power is introduced in the process then there are two menu options available in the ***Edit ▸Process Options ▸Resources*** *and* ***Tasks ▸Other Resources.*** *These are the* ***Power Consumed*** *and the* ***Power Generated*** *options. Also power consumed and generated differ by their properties too.*

6.9c Power Types in Database Sites

To add, edit or delete power declared as utilities in sites, select **Databanks ▸ Sites and Resources** from the main menu. From the Sites & Resources Databank Dialog that appears, you can select the desired site from the left pane (site tree) and the Power node on the right pane and you may add new, edit, or delete power by clicking on the appropriate button from the toolbar.

When adding a new site power you will be presented with a dialog which displays all currently available power types in the databank. From there you can select one or more power types that you want to include in the site.

Once a new power type is added to a site as a site power then you cannot delete it from the power type databank; first you must remove the power type from the site.

If a section is allocated to a site, then available to operations of this section are not only power of this site but of its parent sites as well. This implies that if there is a central power plant in a site then all produced types of power are available to all sub-facilities within that site.

Changes made in site power (i.e. power types associated with sites) may affect existing process files that contain sections that use them. SuperPro Designer will not automatically adjust any files that are currently not open. However, it will require that open process files become consistent with the (updated) information currently available in the site and resources databank. Therefore, all changes done in the site-power databank will automatically be propagated to open process files even if de-allocation (i.e. substitution with generic-type power) is needed to maintain consistency. Such changes could affect economic results so re-doing economic calculations might be needed for all affected process files.

For more details, see 15.8b Adding or Deleting a Power Type.

6.9d Power Type Properties

The parameters of a power type as shown in the power types databank are the default parameters that are used the first time any of the processing steps in your process file employs that power type. If you decide to use different values for your specific process file, then you can adjust those parameters without affecting the default values of the power type in the databank, by bringing up the Power Types dialog that appears when you select the **Edit ▸ Process Options ▸ Power Types** option from the main menu, or just the **Resources ▸ Power Types**

option from the flowsheet context menu. The dialog that pops up displays a list with all power types currently employed by the process file.

To view or edit the properties of a power, you should click on the power type's index column to select it and then press the **View/Edit Properties** button ( ). Alternatively you can double-click on the power. The dialog that appears contains the selected power types data organized in three tabs. Changes made through this dialog will only affect the current process file; they will not be stored in the power types databank. If you want the power type in this process file to take up the properties of the power type in the databank (in case they are different) select the power by clicking on the power's index column and press the **Update Properties from DB Record** button ( ). If you want to update the databank's record (power type properties) based on the current process file record press on the **Deposit/Update Record in DB** button ( ).

The properties for a power type that is consumed or generated are:

- **Voltage**: the voltage of electricity may be different from country to country, the default is 110V for USA.
- **Purchasing Price**: how much does the electricity cost to purchase per unit basis (default in kWh)
- **Selling Price**: the selling price of the power which is produced if any.

Other properties which are only available in this process file (do not exist in the power types databank) and are exclusive to power produced from the process are the following:

- **Revenue vs Credit**: the generated power may be considered as revenue or as a credit to the whole operation of the plant. If a power type is a revenue it is included in the total annual revenues, and if it is a credit it may reduce the total annual operating cost of the plant.
- **Recycling**: the generated power can also be reused in the same process therefore reducing the cost of the total power consumed in a plant. The extent of power recycled can be set by setting a percentage in the relevant edit box.

The **Availability Limits** tab lets you define bounds on consumption of this power type. There are two types of limits: rate limits (instantaneous or time-averaged over a user-defined time span) and cumulative limits over a user-defined time span. Upon request, these limits will be plotted on the resource consumption charts (see 6.10a Power Demand & Power Generation Chart) so that you can compare them against the actual consumption.

Note that, for site power, data in the Properties and Availability Limits Tab are not editable through the Power Currently in Use dialog. The reason is that site power could be shared by different process files and only through the site databank their properties can be modified. To edit those values, you will need to visit the sites databank through the **Databanks ▸ Sites & Resources** menu item as explained before.

The locations (Consumption or Production) where a selected power is currently utilized in the process can be viewed by clicking on the button .This can be in operations or sections.

For more details on the interfaces please see:

- List of Power Types Currently Consumed by the Process
- List of Power Types Currently Generated by the Process
- Power Type Properties Dialog

6.10 POWER CHARTS & TABLES

6.10a Power Demand & Power Generation Chart

You can view in a chart the detailed rate of consumption for a given power type by selecting **Charts ▸ Power ▸ Demand ▸ Single Batch** (Power Demand Chart (Single Batch)) or **Charts ▸ Power ▸ Demand ▸ Multiple Batches** (Power Demand Chart (Multiple Batches)) from the main menu of the application. In a continuous process that contains batch procedures the same chart can be displayed by selecting **Charts ▸ Power ▸ Demand ▸ Selected Time Horizon** from the main menu. Before the chart is presented, you will be prompted to choose a power resource amongst all power resources. Optionally you may specify what to see on the chart and edit the style of the chart.

Besides the actual consumption rate curve, users can chose to see at on the same chart the following lines:

1. A time-averaged consumption rate line (averaged over a user-specified periodic window); for example, users may be interested in seeing the consumption rate of a given buffer in 8-hour average values.
2. A cumulative amount line: Amount total may be of interest when considering inventory capacity. Users may also specify a time period after which the accumulated amount gets reset to 0.0.

The style of the consumption chart dictates exactly which lines will be plotted. As part of the chart's style you can also specify the rate units and the amount units to be used for the chart, as well as the visual characteristics of the lines (color, thickness, etc.) The time-line parameters used (absolute vs relative time scale, minor/major intervals & gridmarks, etc.) are, by default, those kept by the process document. They can, of course, be customized for the consumption charts if needed. the chart's style can be changed through the Power Chart Style Dialog.

The unit choices for plotting rates and cumulative amounts are 'remembered' by the application in association with the power resource being plotted. In other words, you can specify a set of units to be used when viewing power-A (e.g. kW for rate and kW-h for amounts) and a different set of units to be used when viewing power-B (e.g Watt and kcal). On the other hand, the rest of the properties of the graph style (line characteristics, time line properties, etc.) will be used for all power charts (regardless of the power resource chosen).

For the basic common services offered by all time charts (setting the number of batches, zooming in/out, adjusting the time scale, copying the chart as picture, copying chart data to Excel, printing, etc.), see 6.6a Material Consumption & Material Output Charts.

The counterparts of demand charts are the output charts. Such charts available only if there is a power generating procedure in the process. The output charts can be generated by selecting **Charts ▸ Power ▸ Output ▸ Single Batch** (Power Output Chart (Single Batch)) or **Charts**

▸ **Power** ▸ **Output** ▸ **Multiple Batches** (Power Output Chart (Multiple Batches)) from the main menu of the application. Also in a continuous process that contains batch procedures the same chart can be displayed by selecting **Charts** ▸ **Power** ▸ **Output** ▸ **Selected Time Horizon** from the main menu. Before the chart is presented you will be prompted to choose a power resource.

Just as in the case of consumption charts, besides the rate curve, you can choose to include a time-average rate curve and/or a curve tracking the cumulative amount produced. The settings for which lines included in the chart along with visual choices for the lines as well as the time-line characteristics are all part of the style of the chart. The chart's style can be edited through the Power Chart Style Dialog.

6.10b Power Demand Table

The process keeps a detailed log of all power resources present. If you wish to have a direct view of all the power types present currently, you can open the process explorer and pick the 'Util' tab of the Process Explorer Toolbar. This tab will present a quick reminder of all the power resources registered.

If you are interested in seeing the total demand for powers then you should visit the dialog shown when you select **Resources** ▸ **Power Consumed.** from the flowsheet's context (right-click) menu or **Tasks** ▸ **Other Resources** ▸ **Power Consumed** from the application's menu. The List of Power Types Currently Consumed by the Process that comes up will itemize all power types currently registered in the process, their total demand (per batch or per year), their price and total cost.

If you are interested in tracking down the locations and rates where a given power resource is being consumed, then select **Resource Demand Breakdown** ▸ **Power** from the application's main menu. This will bring up the Power Demand Breakdown dialog that presents in a tree-like view (with top nodes each power) the demand for each power and how all the exact sources where they are needed.

6.10c Power Production Table

In order to view total outputs for power resources generated by the process, please visit the dialog shown when you select **Resources** ▸ **Power Generated** from the flowsheet's context (right-click) menu or **Tasks** ▸ **Other Resources** ▸ **Power Generated** from the application's menu. This will bring up the List of Power Types Currently Generated by the Process that presents in a list all generated power types currently registered in the process, their total output (per batch or per year) and their selling price or waste treatment cost.

6.11 LABOR

Every operation requires labor to be carried out. The specification of labor requirements for every operation is done through the Operations Dialog: Labor, etc Tab. Labor requirements can also be defined on a section basis for operation-independent tasks (Operating Cost Adjustments Dialog: Labor Tab and Operating Cost Adjustments Dialog: Lab/QC/QA Tab). SuperPro

Designer keeps track of the instantaneous as well as the cumulative labor demand of the process.

6.11a Definitions in System DB and User DB

The program maintains a (currently limited but easily extended by the user) list of options for labor types that can be used whenever labor demand is required (see 15.9 Labor Types Databank). To review the list of such available labor types, select **Databanks ▸ Labor Types** from the main menu (or hit **Shift + F3** as a shortcut). You can extend the list of available labor types, by adding more to your labor databank (and saved as part of your 'User' database). Changes made in the labor types databank do not affect existing process files or other parts of the databank even if the edited labor types are used as the basis for labor declared in sites.

6.11b Labor Types Currently Used by the Process

In selecting a labor type for an operation or section, you can choose from a list of generic-type labor defined in the databank or, for operations or sections carried out in allocated sites (see 'Section Allocation' on page 8-6), from the corresponding site labor. Labor types currently in use can then be inspected from the List of Labor Types Currently Used by the Process dialog, accessed by selecting **Edit ▸ Process Options ▸ Resources ▸ Labor Types** or **Tasks ▸ Other Resources ▸ Labor Types** from the main menu. From here you may edit the properties of a labor (see 6.11d Labor Type Properties).

6.11c Labor Types in Database Sites

To add, edit, or delete labor declared in sites, select **Databanks ▸ Sites and Resources** from the main menu. From the Sites & Resources Databank Dialog interface that appears select the desired site from the left pane (site tree) and the labor node on the right pane and you may add new, edit, or delete labor by clicking on the appropriate button from the toolbar. In the same way and for each labor site added you may also add specific staff members, who are responsible in carrying out the required tasks.

When adding a new site labor you will be presented with the Add Labor Type Dialog which displays all currently available labor types in the databank. From there you can select one or more labor resources that you want to include in the site.

Once a new user-defined labor is added to a site then you cannot delete it from the labor type databank; first you must remove the labor from the site.

If a section is allocated to a site, then available to operations of this section are not only labor/staff of this site but of its parent sites as well. This implies that labor/staff belonging to a site are available to all sub-facilities within that site.

Changes made in site labor may affect existing process files. Even though SuperPro Designer will not attempt to reconcile process files currently residing in files (but not open by the application), it will require to enforce consistency in any process files that are currently open (when the site-related changes are confirmed). Therefore, all changes done in the site-labor databank will automatically be propagated to open process files even if de-allocation (i.e. substitution with generic-type labor/staff) is needed to maintain consistency. Such changes could affect economic results re-doing economic calculations might be needed for all affected process files.

6.11d Labor Type Properties

The parameters for labor type as shown in the labor types databank are the default parameters that are used the first time any of the processing steps in your process file employs that labor type. If you decide to use different values for your specific process file, then you can adjust those parameters without affecting the default values in the databank, by bringing up the List of Labor Types Currently Used by the Process dialog that appears when you select the **Edit ▸ Process Options ▸ Labor Types** option from the main menu or just the **Resources ▸ Labor Types** option from the flowsheet context menu. The List of Labor Types Currently Used by the Process that pops up displays a list with all labor types currently employed by the process file. To view or edit the properties of a labor type, you should click on the corresponding index column to select it and then press the **Edit** button ( ). Alternatively you can double-click on the labor's index column. The Labor Type Properties Dialog that comes up contains the labor data organized in tabs. If you want a labor in this process file to take up the properties of the same labor in the databank (in case they are different) select the labor by clicking on the labor's index column and press the **Update Data from DB** button ( ) If you change the properties of a labor in this process file and you want them to be stored in the user's database select the labor by clicking on the labor's index column and press the **Deposit /Update Data into DB** button ( ).

The **Properties** tab lets you specify economic data that will be used to calculate the labor cost per hour. These data include a basic rate (in $/hr) along with benefits, supervision, operating supplies and administration factors, or a comprehensive lumped rate (in $/hr). The selection of what option (itemized or lumped) to use is done at the section level of every process file so it is recommended that you provide meaningful values for all cost data.

The **Availability Limits** tab lets you define bounds on the availability of this labor type. There are two types of limits: rate limits (instantaneous or time-averaged over a user-defined time span) and cumulative limits over a user-defined time span. Upon request, these limits will be plotted on the resource consumption charts (see 6.12a Labor Requirement Chart) so that you can compare them against the actual labor need. Note that for staff there is an inherent availability rate limit of 1 labor-hr/hr and a cumulative limit that cannot exceed its defined time span, e.g. a person cannot deliver more than 24 labor hours within a day.

Site labor and staff data are not editable through the List of Labor Types Currently Used by the Process dialog. The reason is that site labor could be shared by different process files and only through the site databank their properties can be modified. To edit those values, you will need to visit the sites databank through the **Databanks ▸ Site and Resources** menu item. As with site utilities, if site labor data are modified, changes are propagated to all open process files that use them in order to maintain consistency with the databank.

The locations where a selected labor is currently employed in the process can be viewed by clicking on the button .This can be in operations or sections, which are displayed in order of first use.

6.12 LABOR CHARTS & TABLES

6.12a Labor Requirement Chart

You can view in a chart the detailed rate of consumption for a given labor by selecting **Charts ▸ Labor ▸ Single Batch** (Labor Demand Chart (Single Batch)) or **Charts ▸ Labor ▸ Multiple Batches** (Labor Demand Chart (Multiple Batches)) from the main menu of the application. In a continuous process that contains batch procedures the same chart can be displayed by selecting **Charts ▸ Labor ▸ Selected Time Horizon** from the main menu. Before the chart is presented, you will be prompted to choose a labor resource type from a list of currently employed labor.

Besides the actual consumption rate curve, users can chose to see at on the same chart the following lines:

1. A time-averaged consumption rate line (averaged over a user-specified periodic window); for example, users may be interested in seeing the consumption rate of a given labor resource in 8-hour average values.
2. A cumulative amount line: Amount total may be of interest when considering labor availability. Users may also specify a time period after which the accumulated amount gets reset to 0.0.

The style of the requirement chart dictates exactly which lines will be plotted. As part of the chart's style you can also specify the rate units and the amount units to be used for the chart, as well as the visual characteristics of the lines (color, thickness, etc.) The time-line parameters used (absolute vs relative time scale, minor/major intervals & gridmarks, etc.) are, by default, those kept by the process document. They can, of course, be customized for the consumption charts if needed. The chart style can be changed from the Labor Chart Style Dialog.

For the basic common services offered by all time charts (setting the number of batches, zooming in/out, adjusting the time scale, copying the chart as picture, copying chart data to Excel, printing, etc.), see 6.6a Material Consumption & Material Output Charts.

6.12b Labor Requirement (Demand) Tables

The process keeps a detailed log of all labor present. If you wish to have a direct view of all the labor present currently, you can open the process explorer and pick the 'Labor' tab of the Process Explorer Toolbar. This tab will present a quick reminder of all the labor registered in the process.

If you are interested in seeing the total demand for labor then you should visit the dialog shown when you select **Resources ▸ Labor Types** from the flowsheet's context (right-click) menu or **Tasks ▸ Other Resources ▸ Labor Types** from the application's menu. The List of Labor Types Currently Used by the Process that appears will itemize all labor resources currently in use in the process, their direct and total demand (per batch or per year), their adjusted basic and lumped price and total cost.

If you are interested in tracking down the locations and rates where the labor resources is employed, then select **Resource Demand Breakdown ▸ Labor** from the application's main menu. This will bring up the Labor Demand Breakdown dialog that presents in a tree-like view

(with top nodes each labor type) the demand for each labor and how all the exact sources where they are needed.

6.13 MATERIAL STORAGE UNITS

A material storage unit can be used to supply material or receive (collect) material. There main purpose is to track the consumption or production of material at specific points in the process. For information on how to create storage units in the process, see Registered (in use) Material Storage Units.

- **Supply Storage Units**

  Supplying storage units may deliver material directly to any bulk input streams. This will basically initialize the contents of the input stream. Certain operations can also utilize supplying storage units in order to bring material in to the hosting equipment by not using a physical stream of the process (stream represented by a line in the flowsheet).

- **Receiving Storage Units**

  Receiving storage units are used to collect material directly from any bulk output streams. Certain operations that don't output material on physical streams of the process may also use receiving storage units to deposit their material. Finally procedures may dump the contents of shared equipment to receiving storge units.

More specifically Material storage units may be used in the following ways:

Supplying Storage Units Usage:

- Bulk Streams (Input): The contents of a bulk input stream can be initialized from a storage unit. The assignment of a supply unit to an input stream is done through the Assign Storage Unit Dialog.
- Gas Sweep Operation: The gas sweep operation requires a sweeping agent which can be provided from a material storage unit.
- Pressurization Operation: This operation requires a pressurization gas to be carried out, the material that the gas is composed of can come from a storage unit.
- Purging / Inerting Operation: The purging gas of this operation can originate from a storage unit.
- Cake Drying (in a Nutsche Filter) Operation: The cake drying operation in a nutsche filter can optionally carry out a gas sweep during drying, requiring a gaseous material which can be supplied by a storage unit.
- In-Place-Cleaning (CIP) Operation: The CIP steps of an In-Place-Cleaning (CIP) operation can optionally obtain the cleaning agent from a material supply unit.

Receiving Storage Units Usage:

- In-Place-Cleaning (CIP) Operation: The CIP steps of an In-Place-Cleaning (CIP) operation can deposit the cleaning agent they use in to a receiving storage unit. Optionally one of the CIP steps can also remove the remaining contents of the vessel as waste together with the disposed cleaning agent, and deposit them in the storage unit.
- In-Place-Steaming (SIP) Operation: The SIP operation can deposit any material that is associated with the Heat Transfer Agent it uses, into a receiving storage unit. Optionally it can also remove the contents together with the utility material, and deposit it in the storage unit.
- Sampling Operation: The amount of material removed for sampling purposes can be deposited as waste in a storage unit.
- Local Receptacle & Automatic Emptying of Contents: When an equipment is shared by more than one procedure, its leftover contents may be emptied as waste before it is re-used. This leftover material may be deposited in a receiving storage unit.
- Bulk Streams (Output): The contents of a bulk output stream can be deposited in a storage unit. It is required that both output stream and receiving storage unit have the same classification. The assignment of a receiving unit to an output stream is done through the Assign Storage Unit Dialog.

Once a storage unit (supply & receiving) are associated with a stream or an operation, then the storage unit is the one that defines the material for supplying units or the classification, treatment/selling price for receiving units. The composition in input streams and the classification of output streams cannot be changed. All options in operation which are related to the associated storage units are disabled.

TRACKING MATERIAL AMOUNTS

Using storage units you may designate the tracking of the consumption or production of material to specific points in the process. This way it is possible to assess how much of a material is required or outputted by a particular operation, unit procedure or section in the process.

The demand in the amount supplied by a storage unit is calculated by the operations that consume the material. Similarly the operations or procedures (if procedure is set to dump leftover contents of equipment before re-use) will also define the total amount of materials that are outputted to receiving units. SuperPro Designer keeps track of the instantaneous as well as the cumulative amounts of material that the storage units may supply or receive.

6.13a Registered (in use) Material Storage Units

New storage units can be registered in a process file by selecting **Edit ▸ Process Options ▸ Resources ▸ Material Storage Units** or **Tasks ▸ Other Resources ▸ Material Storage Units** from the main menu or **Resources ▸ Material Storage Units** from the flowsheet's context menu. From the Material Storage Units Dialog interface that appears you may:

- *Create* supplying units or receiving units through separate tabs by clicking on the **Add** button ( ). You will presented with a dialog that allows you to enter the property data for the creation of a new material storage unit.
- *Edit* the properties of storage units by clicking on the **View/Edit** button ( ). You will be presented with the same dialog used for adding a new material storage unit.
- *Delete* storage units by clicking on the **Delete** button ( ).

See 6.13b Material Storage Unit Properties for details on the various properties of supply and receiving material storage units.

In order to make use of a storage unit you must visit the available usage points (streams, operations or unit procedures) as mentioned previously in the Material Storage Units, and select the appropriate storage unit from a list of registered supplying or receiving units. Please note that when selecting a supplying unit this will change the composition of the input stream or the inputted material of the operation, to the composition of the supply unit. And when selecting a receiving unit you will only have the option to select a receiving unit which is compatible by classification. For example you can not associate a CIP step with a receiving unit whose classification is revenue, the CIP step may only remove the contents as waste.

6.13b Material Storage Unit Properties

The parameters of a storage unit can be inspected or edited by choosing the supply or receiving tab from the Material Storage Units Dialog interface accessed by selecting **Edit ▸ Process Options ▸ Resources ▸ Material Storage Units** or **Tasks ▸ Other Resources ▸ Heat Transfer Agents** from the main menu or **Resources ▸ Material Storage Units** from the flowsheet's context menu.

To view or edit the properties of a storage unit you should click on a storage unit index row to select it and then press the **Edit** button ( ). Alternatively you can double-click on the storage unit row. The dialogs that comes up contains the supplying or receiving units data respectively organized in four tabs.

SUPPLY UNIT PROPERTIES

The properties tab for a supply unit (List of Material Supply Storage Units Tab) lets you define the name of the supply unit, the material supplied, whether the basis is per mass or volume and the density to convert between mass and volume. The density is not the density of the material but the density in the storage unit. This may differ from the density of the material in the associated input stream or operation. The material cost and units displayed is the cost and units of the registered pure component or stock mixture.

RECEIVING UNIT PROPERTIES

The properties tab for a receiving unit (List of Material Receiving Storage Units Tab) lets you define the name of the receiving unit, the classification of the deposited material, whether the basis is per mass or volume and the density to convert between mass and volume. Again the density is not the density of the deposited material but the density in the storage unit. A receiving unit may accept different pure components and/or stock mixtures. You may optionally specify the selling price (revenue or credit classifications) or waste treatment cost (waste classification) and the basis units.

The **Availability Limits** tab lets you define bounds on consumption or exiting material of a storage unit. There are two types of limits: rate limits (instantaneous or time-averaged over a user-defined time span) and cumulative limits over a user-defined time span. Upon request, these limits will be plotted on the resource consumption charts (see Material Supply & Receiving Unit Rate Charts) so that you can compare them against the actual consumption.

The **Inventory Data** tab lets you define storage and supply data of the material in a storage unit, in turn, it will be used to calculate the inventory chart lines (see 6.14b Material Supply & Receiving Inventory Charts). See also 6.5d Material Inventory.

The locations where a storage unit is currently utilized in the process can be viewed by clicking on the button . This can be in operations or streams (input or output), which are displayed in order of first use accompanied with their hosting procedure.

Finally the evolving composition of the contents of a receiving unit, as several material deposits would come in the span of a complete process batch execution, can be viewed by clicking on the button .

6.14 MATERIAL STORAGE UNITS CHARTS

6.14a Material Supply & Receiving Unit Rate Charts

You can view in a chart the detailed rate of consumptions for a given material supply unit by selecting **Charts ▸ Storage Unit ▸ Supply ▸ Single Batch** (Supply Unit Material Demand Chart (Single Batch)) or **Charts ▸ Storage Unit ▸ Supply ▸ Multiple Batches** (Supply Unit Material Demand Chart (Multiple Batches)) from the main menu of the application. In a continuous process that contains batch procedures the same chart can be displayed by selecting **Charts ▸ Storage Unit ▸ Supply ▸ Selected Time Horizon** from the main menu. Before the chart is presented, you will be prompted to choose a storage unit amongst all registered supply units. When selecting the storage unit the material supplied will be shown in a separate field in the dialog. The consumption of this material will be plotted in the chart.

The chart is identical to the material consumption chart, only now you will not see all the consumption points in time but only the consumption points that correspond to the points where the storage unit supplies this material.

The counterparts of the material supply chart are the material deposit (output or receiving) charts. Such charts are of particular importance when tracking waste and waste amounts (e.g. emissions) at receiving points of this material. The material deposit charts can be generated by selecting **Charts ▸ Storage Units ▸ Receiving ▸ Single Batch** (Receiving Unit Material Deposit Chart (Single Batch)) or **Charts ▸ Storage Units ▸ Receiving ▸ Multiple Batches** (Receiving Unit Material Deposit Chart (Multiple Batches)) or **Charts ▸ Storage Unit ▸ Receiving ▸ Selected Time Horizon** from the main menu of the application. Before the chart is presented you will be prompted to choose a storage unit amongst all registered receiving units. Optionally you may also select to plot a single component amongst all components which may have been deposited in the receiving storage unit.

For more details regarding the material consumption and output charts please see 6.6a Material Consumption & Material Output Charts.

The settings for which lines included in the chart along with visual choices for the lines as well the time-line characteristics are all part of the style of the chart. This can be changed through the 6.15ad Material Chart Style Dialog.

6.14b Material Supply & Receiving Inventory Charts

When considering the supply of a material, it is often of importance to design inventory capacity and/or select a preferred replenishing rate so that the process never runs out of material and at the same time, excessive amounts of storage are avoided. SuperPro Designer will not design the inventory system for you automatically. The time-averaged consumption rate curve and time-reset cumulative curve presented on the material supply unit chart provide good clues on what should be your targets for replenishing rate and storage capacity correspondingly, see 6.14a Material Supply & Receiving Unit Rate Charts. However, it is up to the user to provide the application with a suggested inventory strategy then the application can generate an inventory chart that will show material supply unit amounts in the holding tank during one or several overlapping batches. The following inventory information needs to be specified before an inventory chart is generated:

1. Storage capacity
2. Initial contents
3. Lower & upper limits on storage capacity (if anything other than 0% and 100%)
4. Supply (replenishing) rate
5. Supply (Replenishing) policy: Need a start time when policy activates and an on/off triggering mechanism (either tied to inventory level or tied to a regularly timed schedule).

For more details on the inventory parameters, see Entering or Exiting Material Dialog: Inventory Data tab.

You can view inventory charts by selecting **Charts ▸ Storage Units ▸ Supply Inventory ▸ Single Batch** (Supply Unit Material Inventory Chart (Single Batch)) or **Charts ▸ Storage Units ▸ Supply Inventory ▸ Multiple Batches** (Supply Unit Material Inventory Chart (Multiple Batches)) from the application's main menu. In a continuous process that contains batch procedures the same chart can be displayed by selecting **Charts ▸ Storage Unit ▸ Supply Inventory ▸ Selected Time Horizon** from the main menu.

For the basic common services offered by all time charts (setting the number of batches, zooming in/out, adjusting the time scale, copying the chart as picture, copying chart data to Excel, printing, etc.), see 6.6a Material Consumption & Material Output Charts.

Similar inventory charts can be generated for the receiving storage unit, by selecting **Charts ▸ Storage Units ▸ Receiving Inventory ▸ Single Batch** (Receiving Unit Material Inventory Chart (Single Batch)) or **Charts ▸ Storage Units ▸ Receiving Inventory ▸ Multiple Batches** (Receiving Unit Material Inventory Chart (Multiple Batches)) or **Charts ▸ Storage Unit ▸ Receiving Inventory ▸ Selected Time Horizon** from the application's main menu. This time, besides selecting a pure component, the user must also provide a holding capacity and a removal strategy (essentially the same items of information as for the supply inventory above, items 1 through 5).

6.14c Material Storage Unit Tables

The process keeps a detailed log of all storage units present. If you wish to have a direct view of all the storage units present currently (supply & receiving), you can open the process explorer and pick the ‘SU’ tab of the Process Explorer Toolbar. This tab will present a quick reminder of all the supplying and/or receiving storage units registered.

7 SCHEDULING

Process scheduling deals with the timing of operations in batch processes. SuperPro Designer provides several means for specifying the start times and durations of operations; it also features several charts for viewing the resulting schedule for either a single batch or multiple batches in a single product campaign. It must be noted that SuperPro Designer will not automatically resolve any scheduling conflicts by taking action and modifying the proposed schedule nor will it propose a complete and realizable schedule that will optimize a user's objective and at the same time avoid any resource constraints. Instead, SuperPro Designer will detect any scheduling conflicts (equipment sharing violations or resource consumption violations) and present several charts that depend on the proposed schedule that will help the user visualize the problematic part of the schedule and allow him/her to propose a solution. There are several interfaces that allow the user to easily modify key scheduling parameters as well timing inter-dependencies and quickly view the results on the overall process schedule. All such interfaces can be accessed either from the process flowsheet or from the various time charts that are presented. Before we explain the scheduling calculations and how the results are presented, users need to understand the scheduling terminology as used by the application (see 7.1 Scheduling Terms & Definitions). The overall schedule depends on decisions and variable values that can be set at the operation level, procedure level or process level (see 7.2 Scheduling Data). The scheduling engine always runs after the mass and energy (M&E) balance calculations are executed as some of the inputs to the calculations (e.g. operation durations) may be calculated at the end of M&E balance calculations. The results of the scheduling calculations (see 7.3 Scheduling Calculations) can be viewed on the Recipe Scheduling Information Dialog or on charts that depict the overall process schedule for operations (see 7.4 The Operations Gantt Chart (OGC)) or equipment (see 7.5 The Equipment Gantt Chart (EGC)). Time utilization of auxiliary equipment (e.g., CIP skids) (see 6.4 Auxiliary Equipment Charts & Tables) or other resources such as labor (see 6.12 Labor Charts & Tables), materials (see 6.6 Material Charts & Tables) or heat transfer agents (see 6.8 Heat Transfer Agent Charts & Tables) can also play an important role in adjusting the scheduling of the process.

7.1 SCHEDULING TERMS & DEFINITIONS

Procedure Cycle: the once through execution of all operations in the procedure's queue (one after another as specified by the user on The Operation Sequence Dialog).

Procedure Cycle Duration: the amount of time it takes for single procedure cycle to complete. The procedure cycle duration is always calculated as the time lapsed between the start of the first operation in the queue and the end of that the last operation in the queue. Note

that this time may not be equal to the sum of all operation times in the queue as some operations' timing may overlap others in the procedure (e.g. stir while heating) or there may be gaps between the end of one operation and the start of the next.

Procedure Cycle Time: the amount of time between consecutive starts of a procedure cycle. Is meaningful if the procedure is repeated cyclically multiple times (Number of Cycles > 1) during a single batch.

Number of Cycles (per batch): the number of times a procedure's cycle is repeated during the processing of a single batch amount.

Number of Cycles (per main recipe cycle): the number of times a procedure's cycle is repeated during the processing of the main recipe cycle time.

Procedure Time: the total amount of time it takes for a procedure to be completed. It is equal to the product of the Number of Cycles times the Procedure Cycle Duration. If the procedure has only one cycle, then the procedure time and the procedure cycle duration are the same.

Setup Time: the amount of time (per cycle) spent before each operation is carried in preparation for the actual execution of the operation. It may involve actions like cleaning, vacuuming, setting up of equipment, etc. which the user opted not to model explicitly.

Process Time: the amount of time (per cycle) during which the actual processing is done. The process time is either specified by the user or calculated by the program.

Turnaround Time: the amount of time (per cycle), that the operation's equipment is being prepared for the next cycle (cleaning, transferring of material, sterilization, etc. that is not explicitly modeled but simply lumped up as part of the operation's cycle time).

Operation Cycle Time: the amount of time it takes for an operation's cycle to be performed. The Operation Cycle Time is the sum of the Setup Time, Process Time and the Turnaround Time.

Start Time Shift: the time elapsing between the start of an operation and a reference point in time. The reference point can be:

(a) the start of the batch

(b) the end (or start) of the previous operation (whatever may be) in the sequence

(c) the end (or start) of another (named) operation in the same procedure

(d) the end (or start) of another (named) operation in another procedure

Start Time Reference Operation: if the Start Time of an operation is not defined with respect to the start of the batch (absolute start time), then it is defined with respect to another reference operation (the Start Time Reference Operation). Note that the start time of an operation can be specified either with respect to the start or with respect to the finish of a start time reference operation.

Absolute Start Time: assuming the earliest operation in a batch starts at time 0, the absolute start time of an operation (or procedure) is the amount of time that elapsed since the beginning of the batch before this operation (or procedure) started executing. If the operation is part of a procedure with multiple cycles, the absolute start time refers to the start of the operation as part of the first cycle of the procedure.

Absolute End Time: assuming the earliest operation in a batch starts at time 0, the absolute end time of an operation (or procedure) is the amount of time that elapsed since the beginning of the batch before this operation (or procedure) ended executing. If the operation is part of a procedure with multiple cycles, the absolute end time refers to the end of the operation as part of the last cycle of the procedure.

Hosting Equipment or Container Equipment: the equipment resource engaged during the execution of the procedure. Remember that every icon shown on the flowsheet represents a procedure (and not equipment) that executes in a container equipment resource that may involve one (or more) pieces of equipment (transportation procedures present an exception since they have no associated process equipment).

Equipment Sharing: In a batch process it is common to utilize the same equipment resource for carrying out multiple procedures (equipment sharing). This is particularly common for storage when handling mixing of materials, heating, cooling, reaction, evaporation, extraction, crystallization, etc. By default, whenever a procedure is introduced in the process, the system assumes that the procedure is carried out in its equipment resource and therefore it creates one automatically for it. After the procedure is created, you can assign a pre-existing equipment resource to it (see 6.1b Equipment Selection & Sharing).

Equipment Cycle Time (aka equipment occupancy time): the time lapsed between the start of the first procedure utilizing this equipment resource and the end of the last procedure utilizing the same equipment in the span of a single batch execution. Please note that this may not be equal to the sum of procedure times (if multiple procedures are hosted) as there may be time between procedure engagements (waiting time). If the equipment hosts only one procedure, then the equipment cycle time equals its hosting procedure time.

Equipment Busy Time: the total time that the equipment resource is engaged in hosting a procedure. If the equipment resource is hosting only one procedure, then the busy time is the same as the cycle duration (and the procedure's time). If the equipment resource hosts multiple procedures, then the equipment busy time is the sum of all procedure times hosted by the resource.

Scheduling Bottleneck Equipment: the equipment with the longest cycle time. The scheduling bottleneck equipment determines the minimum recipe cycle time and the maximum possible number of batches per year (see below).

Holdup Time: when a batch (cyclical) procedure, (e.g., chromatography) operates in a continuous process, the application assumes that the procedure processes material continuously fed to it and accumulated over a period of time called the holdup time. Typically the holdup time is specified by the user. The specified value of holdup time must be greater or equal to the cycle time of the batch procedure. For more details, see 5.2a Holdup Time.

Annual Operating Time Available: the amount of time per year that all equipment and resources are assumed to be available for running this process.

Utilized Annual Operating Time: the actual amount of time per year that all equipment and resources where engaged to run this process (may be less than the available annual operating time).

Recipe Batch Time: the time elapsing from the start of the first cycle of the first (earliest scheduled) operation to the end of the last cycle of the last (latest scheduled) operation required to carry out a single batch.

Recipe Cycle Time: the time between the start of two consecutive batches. It is always smaller or equal to the Recipe Batch Time and larger or equal to the Minimum Recipe Cycle Time (see below). If a batch is started right after the previous one is ended (but not before) then the cycle time equals the batch time. If a batch is started before the previous batch is ended (more typical) then the cycle time is less than the batch time. Note that there is a constraint as to how soon we can start a batch (while the previous is still in progress).

Minimum Recipe Cycle Time: the minimum time possible between the start of two consecutive batches. It is equal to the longest Equipment Cycle Time amongst all equipment resources (excluding those that are ignored by the scheduling calculations).

Recipe Cycle Time Slack: The difference between the recipe cycle time and the minimum recipe cycle time (must always be positive). To maximize the number of batches per year, the cycle time slack should be 0.0.

Maximum Number of Batches: the maximum Number of Batches possible to be processed in a calendar year (without violating the available annual operating time). This Number of Batches can be achieved when the process operates under the Minimum Cycle Time (or the Cycle Time Slack is 0.0).

Number of Batches Per Year: the number of times a batch can be processed in a calendar year (within the available operating time window for this recipe).

Campaign: a string of uninterrupted batch executions (of the same recipe) during a calendar year. Oftentimes, a specific product produced in batch, is produced annually in several campaigns. During the time between campaigns for this product, the equipment is utilized for the execution of recipes leading to other products.

Number of Campaigns: the number of uninterrupted sequences of batches produced each year.

7.2 SCHEDULING DATA

Data that may affect the overall process schedule can be specified at the:

(a) Operation Level (e.g. start time shift, setup time, etc.)

(b) Procedure Level (e.g. number of cycles)

(c) Recipe (or Process) Level (e.g. available annual operating time, cycle time slack, etc.)

MODE OF OPERATION FOR THE ENTIRE RECIPE/PROCESS

Depending on how you intend to operate your process, you may set the operating mode to either batch or continuous (see also 8.14d Process Operating Mode: Batch vs. Continuous). In most cases, the choice is clear. In typical continuous plants all steps are continuous and in typical batch plants all steps are batch. In some cases, a mixed operating environment exists. Some procedures operate in batch (cyclical) mode where there is a down time (or 'off time')

while other procedures may be carried out continuously (i.e. they are 'on' all the time). Typically, the mode by which you produce your main product will dictate your choice for the process operating mode. If the overall operating mode is set to continuous, then no scheduling data are required at any level (operation, procedure or process) and all the Gantt Chart, Equipment Occupancy Chart and Resource Tracking Chart interfaces and menu options are disabled. The overall operating mode of a process is set from the Process Operating Mode Dialog.

7.2a Operation-Level Scheduling Information

For each operation (assuming the overall operating mode is batch) you must specify the following information:

(a) Setup Time

(b) Process Time (sometimes process time is calculated by SuperPro Designer, see Notes below)

(c) Turnaround Time

(d) Start or Finish Time Shift and

(e) Start or Finish Time Reference Operation.

The operation-level scheduling information can always be set from the Operations Dialog: Scheduling Tab even though some of the above parameters may also appear on the 'Oper. Cond's' tab of the operation's i/o simulation dialog.

NOTES:

(a) The process time of an operation could be calculated by the program instead of being set by the user. Typically (but not always) this may be the case when the hosting equipment resource is in rating mode (i.e., its size/capacity is specified). In some operations, the user has the choice instead of setting directly the process time to set some other rate variable (e.g. a transfer rate or a heating/cooling rate, etc.) and allow SuperPro Designer to compute the time required to archive a certain operating goal (e.g. transfer a given amount, or reach a specified temperature). For some purely cyclical unit procedures, such as chromatography, the process time is always calculated. For inherently continuous unit operations (such as pumping) that operate semi-continuously in a batch process, the process time is always specified. Finally, the process time could also be dictated by another operation, if a master-slave relationship is specified (see Note (d) below). In summary, a unit operation's process time (and duration) assumes a value as:
- Set by User,
- Calculated based on other specifications (such as rates, etc), or
- Set by a Master-Slave Relationship.

(b) Specifying the setup time, process time, turnaround time and/or number of cycles may affect the outcome of the scheduling calculations (process batch time, number of batches etc.) as well as some of the simulation results (sizing of process units, capital cost, etc.).

(c) Oftentimes, the timing (duration) of an operation is totally dependent upon the duration of another operation (e.g. the transfer time to a filtration unit is totally regulated by the rate of filtration). In this case, you can establish a **master-slave relationship** between the

two operations: i.e. designate the transfer operation to be the slave of the filtration operation. Having done that, then all three duration parameters of the transfer operation (setup time, process time and turnaround time) will be assumed as equal to the filtration's equivalent times and whenever the filtration parameters change, the transfer operation's parameters will change as well. Even though any operation can be selected as a master operation, not all operations allow the option of becoming a slave operation. If a unit operation's scheduling allows a master-slave relation, it is done through the operation's 'Cond's' tab. There could be multiple options for how the process time of the operation is determined. If setting a master-slave relation is one of them it would appear on that tab and when selected, it will activate a button labeled **Setup**. Clicking on this button, will bring up The Master-Slave Relationship Dialog that allows you to choose the master operation and specify how the master's duration will be used to calculate the duration of the slave.

7.2b Procedure-Level Scheduling Information

The main scheduling information that can be adjusted by the user at the procedure level is the number of cycles and, under certain circumstances, the holdup time. As of version 9.0 when the operating mode of the entire recipe is batch then a procedure may also be set to cycle independently to the recipe and the main batch. Hence the time between consecutive starts of the procedure or the number of cycles per main recipe cycle can be modified as well. All this information can be set through the Procedure Data Dialog: Scheduling Tab (the dialog appears when selecting **Procedure Data** from the procedure's command (or context) menu.)

THE NUMBER OF CYCLES

Setting the number of cycles in a procedure to anything other than 1 implies the following:

(a) the amount of material processed per batch will be divided equally amongst each cycle (thereby reducing the processing load per cycle),

(b) the sequence of operations in that procedure will repeat themselves as many times as the number of cycles (possibly increasing the total procedure time).

For more on the procedure cycle, see 5.2b Procedure Cycle and Cycle Duration.

THE HOLDUP TIME

When a batch procedure (like chromatography, batch filtration, batch distillation, etc.) is set to operate in a continuous process, SuperPro Designer needs to infer the amount of material that gets processed per cycle. In other words, the implicit assumption is that, in order for this procedure to function cyclically in an otherwise continuous environment, there must be a tank that accumulates material for a certain time (at least while the procedure is in progress) and then feed the next cycle of the procedure. This time we call **holdup time** (see also 5.2a Holdup Time).

CYCLE TIME

When the number of cycles of a procedure is greater than one then a cycle time can also be set to indicate the time between the start of two consecutive procedure cycles. This cycle time cannot be less than the cycle duration of the procedure

TIME BETWEEN CONSECUTIVE STARTS (INDEPENDENT CYCLING)

When a procedure is set to cycle independently from the main process than the user can specify the time between consecutive starts of the procedure. By default this time is equal to the main Recipe Cycle Time of the process, but can be adjusted in order for the procedure to be executed as many times as possible within the span of the recipe cycle time.

NUMBER OF CYCLES PER MAIN RECIPE CYCLE (INDEPENDENT CYCLING)

Instead of setting the time between consecutive starts, when the procedure has been set to cycle independently, the user can set the number of times that the procedure is executed during the main recipe cycle time. The number of times the procedure is carried out can be a non integer number as the procedure's cycle durations may not fit exactly in the span of the recipe cycle time.

7.2c Recipe/Process-Level Scheduling Information

The following parameters, as they apply to the entire process, must also be specified:

(a) the Available Annual Operating Time,

(b) the Number of Campaigns and

(c) one of the following: Number of Batches, Cycle Time or Cycle Time Slack.

The recipe-level scheduling information can be set from the Recipe Scheduling Information Dialog accessed by selecting **Tasks ▸ Recipe Scheduling Information** from the main menu.

7.2d Output of Scheduling Calculations

Based on scheduling information provided at all above levels (operation, procedure and process), the scheduling engine of the program will be invoked at the end of M&E balances and it will calculate the following (as outputs, see 7.3 Scheduling Calculations):

(a) the process batch time (aka recipe batch time), BT

(b) the minimum recipe cycle time, CT_{min}

(c) the maximum number of batches per year, NB_{max}

(d) the longest procedure in the recipe

(e) the scheduling bottleneck equipment, and

(f) two out of: number of batches per year (NB), cycle time (CT), cycle time slack (CTS).

The scheduling outputs can be viewed from the Recipe Scheduling Information Dialog accessed by selecting **Tasks ▸ Recipe Scheduling Information** from the main menu.

*Besides updating the scheduling outputs, SuperPro Designer's scheduling engine will also check to make sure that no major scheduling constraints are violated (equipment sharing violations, minimum cycle time violations, etc.). If any such constraint violations are found, they will be reported at the error/warning output window (see 8.17 Error Output Window). Note that the scheduling engine will also be checking for scheduling violations before a request for a time chart is made by the user and after each operation's, procedure's or equipment's i/o simulation dialog is closed. If you wish to have the scheduling violations only be reported after the end of M&E balances, you can visit the flowsheet's preferences dialog (select **Preferences ▸ Miscellaneous** from the flowsheet's context menu, see Miscellaneous Process Preferences Dialog)*

7.3 SCHEDULING CALCULATIONS

All scheduling calculation are performed after the mass and energy balances have been calculated as some of the inputs to the calculations (e.g. operation durations) may be calculated at the end of M&E balance calculations.

7.3a Scheduling Output Calculations

Based on all operation scheduling data (start times and durations) and procedure scheduling data (number of cycles), the application computes all the absolute start and end times for all operations and procedures in the recipe as well as all equipment occupancy times. The latest operation absolute end time defines the batch duration or batch time (BT); the longest equipment occupancy time defines the minimum cycle time (CT_{min}). If there are equipment in the process that are shared and used across batches, then the minimum cycle time may be defined by the longest equipment busy time.

If desired, you can exclude altogether an equipment (and its contained procedures and operations) from any scheduling considerations. For instance, you may not wish to have simple mixers or splitters appear in your Gantt charts. Select ***Equipment Data*** *from the procedure's command menu and from the ensuing dialog check the box indicated by the label* ***Omit from Scheduling****. From then on, any procedures hosted by this equipment resource (and operations included in those procedures) will not contribute to the recipe's batch time and they will not appear in any scheduling related charts (Gantt Chart, Equipment Occupancy Chart, etc.).*

Next, using the recipe's available annual operating time (AOT_{av}), and the annual number of campaigns (k) the system computes the maximum number of batches per year (NB_{max}) using the following relationship:

$$AOT_{av} = (NB_{max} - k)CT_{min} + kBT \qquad \text{eq. (7.1)}$$

Note that the same relationship as shown in eq. (7.1) also holds when AOT (actual) is used instead of AOT_{av} and CT and NB are used instead of CT_{min} and NB_{max}

$$AOT = (NB - k)CT + kBT \qquad \text{eq. (7.2)}$$

The following relation exists between CT, CTS and CT_{min}

$$CT = CTS + CT_{min} \qquad \text{eq. (7.3)}$$

Since the user provides either CT or CTS and CT_{min} is always calculated based on the operation-level scheduling data, we can assume that CT is always available (either as a direct input by the user - in which case the system calculates CTS from eq. (7.3) - or as output of eq. (7.3) using the user-provided value of CTS. Based on the fact that CT is always known, we can use eq. (7.2) two ways:

(a) If the NB is allowed to be calculated, then we calculate NB as the maximum integer that keeps the right-hand of side of eq. (7.2) less than or equal to AOT_{av} (upper limit); with this value of NB, eq. (7.2) is evaluated to provide the actual value of AOT.

(b) If the NB is provided by the user, then we use eq. (7.2) directly to calculate the actual AOT (must be $\leq AOT_{av}$).

7.3b Scheduling Constraints

Before performing any scheduling calculations, SuperPro Designer verifies that no scheduling constraints are violated. Scheduling constraints are checked at:

- Each equipment resource level
- Overall process scheduling level

At the individual equipment resource level, SuperPro Designer will make sure that:

(a) no two procedures have been scheduled to execute using the same equipment host with overlapping procedure times. If you don't employ equipment sharing, then no such constraints at the equipment level will exist.

(b) all operations in a procedure, have (possibly calculated) absolute start times that are consistent with their execution order (in the procedure's queue).

The constraints at the recipe level have to do with the setting of unachievable goals expressed as user specifications at the recipe level.

1. If the user supplied the value of CT, then after CT_{min} is known, the system will make sure that CT is always greater or equal to CT_{min}.
2. If the user provided NB, then we must make sure that NB is always less than or equal to NB_{max}.
3. Finally, if both NB and CT are provided, the application will make sure that the resulting AOT is less than or equal to AOT_{av}.

If any of the above targets lead to a constraint violation, then SuperPro Designer will announce that your scheduling targets may be infeasible (message will be echoed in the error output window).

7.3c Cycle Time Bounds Calculation

As indicated earlier, in the calculation of CT_{min} each equipment contributes its own occupancy time (including both busy and idle intervals) unless the equipment is shared across batches; in this latter case, the longest busy time among all steps that share the equipment is taken into account in the calculation of CT_{min}.

In the absence of equipment shared across batches, CT_{min} is the lowest bound on all feasible cycle times; any implemented cycle time greater than CT_{min} is guaranteed to produce feasible schedules with no equipment conflicts. If, however, there exist equipment (such as CIP skids) that are assumed by default to be sharable across batches or are declared by the user to be sharable, then the calculated, in the above way, CT_{min} is not necessarily feasible and the feasible CT value region is not a continuous interval. For this reason, SuperPro Designer offers a feature that will aid the user in finding all feasible cycle time bounds.

The algorithm implemented in SuperPro Designer for calculating feasible cycle time bounds is based on literature in *cyclic scheduling* and more specifically on the work of Mayer et al. (2008) and Hanen (1994). Very roughly, the calculation process checks all possible pairs of processing steps (procedures or operations) that share the same equipment to identify cycle time bounds that lead to non-overlapping schedules. For any processing steps *i* and *j* with *i* being executed before *j* within a batch, it can be proven that feasible cycle times must satisfy the following relation:

$$\frac{e_j - s_i}{K(j,i)} \le CT \le \frac{s_j - e_i}{K(j,i) - 1} \qquad \text{eq. (7.4)}$$

where s_i is the absolute start time of step *i*, e_j is the absolute end time of step *i* and *K(j,i)* is a positive integer. For different values of *K(j,i)* the above relation yields all possible cycle time intervals that produce schedules where steps *i* and *j* do not overlap across batches. The intersection of all these feasible intervals for all possible pairs of equipment-sharing steps yields the cycle time bounds that make the entire process feasible.

References

1. Hanen C., "Study of a NP-Hard cyclic scheduling problem: The recurrent job-shop", *European Journal of Operational Research*, **72** (1994) p82-101.
2. Mayer E., Haus U-U, Raisch J., Weismantel R., "Throughput-optimal sequences for cyclically operated plants", *Discrete Event Dyn Syst*, **18** (2008) p355-383.

7.3d Scheduling and Equipment Sizing

Process scheduling decisions have an impact on equipment sizing and reversely, equipment sizes have an impact on the process schedule. When equipment resources are set in design mode, longer cycle times for operations lead to longer cycle times for procedures and therefore they may increase the minimum recipe cycle time leading to fewer number of batches per year. Raising the number of cycles in a procedure to values higher than one, may result in smaller equipment capacity demands (which is equivalent to lower capital investment) but at the same time they increase the cycle time of the procedures and therefore the equipment occupancy times, possibly pushing the minimum cycle time to higher values. Such an increase, once again, may lead to fewer feasible number of batches per year, and possibly to a small annual throughput. Sharing of equipment resources by multiple procedures has a potential similar effect: yields a direct savings in capital, but at a potential penalty in NB_{max}. Such trade-offs between capital and throughput will be further analyzed in Chapter 11 (Debottlenecking). When designing new facilities, users should strive for a balance between capital investment, plant capacity, and flexibility for expansion.

7.4 THE OPERATIONS GANTT CHART (OGC)

The operations gantt chart presents an overview of the entire schedule for a single or multiple batches as a Gantt chart. To display the Operations Gantt Chart (Single Batch), select **Tasks ▸**

Gantt Charts ▸ Operations GC. To display the Operations Gantt Chart (Multiple Batches), select **Tasks ▸ Gantt Charts ▸ Operations GC (Multiple Batches)**. Multiple batches may be of interest when there is batch overlapping (i.e. the second batch starts before the first batch, or in other words when the cycle time is less than the batch time).

There are two types of bars in the chart:

- Activity Summary Bars, representing a composite activity, i.e. an activity that can be expanded or refined to other activities, e.g., a procedure.
- Elementary Activity Bars, representing a single, non-expandable activity, e.g. an operation in a cycle.

There are seven levels of activities considered by the operations Gantt chart. Those levels in order of hierarchy are as follows:

1. Batch
2. Branch
3. Section
4. Procedure
5. Cycle
6. Operation

Each task (activity) bar in the above hierarchy expands into subtasks of the level below. Since branches and sections may not often be used in a process simulation, their levels can be optionally skipped; in that case, batch-level activity bars expand directly into procedure bars. You can edit the style of the chart through the Operations Gantt Chart Style Dialog. Different levels can be selected or omitted through the Operations Gantt Chart Style Dialog: Contents Tab. Each bar has its own visual style that can be customized by the user. Users may also find it convenient to display next to each task bar a short description of the activity represented by the bar. You can turn on or off the textual description (perhaps only for certain types of activities, e.g. operations only) by modifying each activity's style.

The operations Gantt chart interface window is divided into two views:

(a) the spreadsheet view (left). The spreadsheet view displays in each line the name, duration, start and end time for each activity whose bar line is shown straight across on the chart (all information is presented for viewing purposes only). You use the left view to expand and/or collapse activity summaries by clicking on the + or - buttons showing at the left of the activity name.

(b) the chart view (right). The chart view displays, as a horizontal bar drawing against the time line, each activity participating in the overall scheduling of the recipe. Right-click on a bar and a relevant command menu will come up. Selecting the first menu entry will bring up a dialog that will allow you to edit scheduling information associated with that particular activity bar. At any time you can request to have the M&E balances redone and to have the Gantt chart updated to reflect the new (calculated) scheduling settings for the recipe. Simply click on the **Update Chart** entry in the main menu of the interface or click on the **Refresh** button of the chart's toolbar. Note that since this command

will re-run the simulation, it may result in the display of several simulation error and/or warning messages generated during simulation.

When you are done working with the Gantt chart interface, you can close it down by selecting the **File ▸ Exit** option from the main menu or simply click on the button (top-right).

DEFAULT NUMBER OF BATCHES

When a multi-batch chart is chosen to be shown, the default number of batches (N_b) shown at first is calculated as follows:

$N_b = 1 + [BT / CT]$, where

[BT/RCT] is the rounded up integer ratio of the recipe's batch time (BT) divided by the recipe's cycle time (CT). The number is chosen this way, so that even if you later view a larger number of batches, all future batch graphs will always have a pattern that can be mapped within this chart (with some offset). In other words, N_b as calculated above, s is the minimum number of batches necessary to plot such that it will capture all possible batch interactions. Of course the number of batches can later be set to any number (select **Set Number of Batches** from the chart's command menu).

SuperPro Designer uses a default coloring scheme for presenting all the occupancy bars belonging to the same batch. This makes it very easy to visually convey the batch number for each activity (task) bar. The legend window at the side of the chart indicates which color has been chosen for each batch ID. The user can modify the color to be used for a given batch ID by simply double clicking on its color sample in the legend window.

TIME LINE

The x-axis represents time. By default, the axis start time is 0.0. In other words, the time value of '0.0' is assigned to the earliest engagement of an equipment (aka beginning of the batch). If so desired, a real date/time can be assigned through the Graph Style Dialog (All Time Charts): Time Line Tab. The time axis displays two lines with increments of time: minor and major. The settings for what time increment to be used for major and minor increments as well as what units to be displayed is also customizable. By default a vertical gridline will be displayed on both minor and major increments but they can be turned off is so desired.

PRINT PREVIEW

You can print (or print preview) a chart directly from SuperPro Designer by selecting the **Print** (or **Print Preview)** command from the chart's command menu. If the printing quality is not adequate, or more printing options are desired (e.g. smarter scaling, etc.) then it is recommended that you export the chart as a picture into another application first (e.g. MS-Excel®) and then print it.

7.4a Accessing Scheduling and Simulation Data

From the operations Gantt chart interface (single or multiple batches) you can access all scheduling and most simulation data for the entire recipe. When utilized in this way, this interface becomes an alternative way to view and work with your recipe. To access the data, you must right-click over a chart's bar, and select the first entry from the command menu that pops up. The menu entry and the ensuing dialog depend on the type of bar you started:

For recipe (batch) summary bars: the Recipe Scheduling Information Dialog allows you to edit the recipe-level scheduling data (annual operating time, number of campaigns, etc.)

For branch summary bars: the Branch Properties Dialog presents all branch properties.

For section summary bars: the Section Properties Dialog presents all section properties.

For procedure summary bars: the Procedure Data Dialog allows you to change the number of cycles for that procedure.

For procedure cycle summary bars: the Cycle Description Dialog presents some cycle-related information (for viewing purposes only).

For operation elementary activity bars: the Operation i/o Simulation Dialog is the same as the dialog that you view from the main interface of SuperPro Designer. It allows you to edit the operating conditions as well as the scheduling settings for that operation.

All changes made through any dialogs invoked during the time the Gantt chart interface is active, are permanent and cannot be reversed (even if you exit the chart by clicking on the *button (top-right).*

7.4b Exporting Chart & Data to Other Applications

EXPORTING THE OGC (AS A DRAWING)

You can copy the chart (as a picture) by selecting **Copy ▸ Chart** and its legend by selecting **Copy ▸ Legend** (the latter only available in multi-batch charts). Then, you can go to another application (e.g. MS-Word®, or MS-Excel®) and issue a paste command. This will paste the chart (or the legend) as a picture in the destination document. Another way of exporting the chart (as a picture) is to save it in a Windows Metafile ('wmf') format in a file and later import the picture file into another application. You can export the chart picture in Windows Metafile Format by selecting **Export Chart as Metafile** from the chart's command menu.

EXPORTING THE OGC'S SPREADSHEET (AS A TABLE / SPREADSHEET)

You can copy the Gantt spreadsheet and paste it into other applications as a table (e.g. in MS-Excel®, MS-Word®, etc.) This can be done by right-clicking on the Gantt spreadsheet area and selecting **Copy Gantt Spreadsheet** from the ensuing menu.

EXPORTING ALL SCHEDULING DATA INTO MS-EXCEL®

The chart's scheduling data can be exported in a tabular format that can be readily imported into MS-Excel® for further processing / plotting etc. You can select **Export Data to Excel** from the chart's command menu and then provide a file name and location, and SuperPro Designer will include the data into the selected file.

EXPORTING ALL SCHEDULING DATA INTO MS-PROJECT®

You can export all the scheduling information into MS-Project® by selecting **File ▸ Export to MS Project XML File...** from the menu of the Gantt chart interface. The exported xml file can then be opened in MS-Project®.

▶ **To import scheduling data into MS Project® (MS Project® 2000 or higher)...**

1. Start MS Project® and select **File ▸ Open**
2. Click on the **ODBC** button
3. Switch to **'**Machine Data Source**'** tab
4. Locate and select **'ProDesigner MS-Project DB'** and click **OK**
5. Locate the name of the project that you just exported and click **OK**.

EXPORTING ALL SCHEDULING DATA INTO SCHEDULEPRO®

SchedulePro is a separate application developed and marketed by Intelligen that handles scheduling and debottlenecking of single and multi-product facilities in detail. Recipes developed in SuperPro Designer can be readily exported to SchedulePro by selecting **File ▸ Export to SchedulePro Recipe DB** from the application's main menu. The recipe data are deposited into a 'Recipe Database' and from there they can be readily imported into SchedulePro. Once imported into SchedulePro users can have a wider flexibility in building single or even multi-product (sharing the same site) campaigns.

7.4c Zooming / Time Scale

The time axis can be either stretched out (in order to view more details of the chart), or condensed in order to manage to fit the chart in a smaller visible region. The three factors that determine how much of the chart will be visible in a given window space are:

1. The viewing mode
2. The time scale chosen for minor & major increments, and
3. The zooming factor

There are two viewing modes: **Fit-to-Window** and **Nominal**. When the graph viewing mode is set to 'Fit-to-Window' (the button is pressed) the application will display the graph's contents always in the available window width. In this mode, a user can gain an overall perspective of the entire graph, at the expense of missing small details. When the chart is viewed in this mode, it is possible that not all of the major and/or minor increments of time can be individually visible. Sometimes, the increments will be melded into two, or three or more at a time, in order for the labels to fit and in order for the entire time span to fit in the available space. In this mode priority is given to displaying the entire graph within the allotted space. In the 'Nominal' viewing mode (the button is pressed) the application decides the scale by which to display the occupancy information in a way that the user's selection for minor increments is obeyed. In other words, in this mode, all the minor increments are displayed, more than likely requiring more horizontal space than what is available in a single window width, so a horizontal scroll is now visible. In that mode, you can further increase or decrease the zooming factor by using the **Zoom to** button (

) or the **Zoom by** button (

)of the toolbar. The **Zoom to** option will pick a zoom factor such that the chart's window will display exactly the selected span of time (a day, a month, etc.). The **Zoom by** option simply increases or decreases the zooming ratio by the selected percentage, thereby

allowing more or less details to be visible on the graph. You can also zoom in and out by selecting the corresponding commands in the chart's command menu.

The zoom in/out and zoom to/by commands and/or buttons on the toolbar are only active if the viewing mode is set to 'nominal'. When viewing the chart in the 'fit-to-window mode', the scale is automatically picked to make sure that the chart fits in the available space.

7.4d Appearance (Visual Style)

The visual appearance of a Gantt chart can be modified through the Operations Gantt Chart Style Dialog. To access that dialog, you can either select **Preferences ▸ Styles ▸ Gantt Chart** from the Gantt Chart main menu, or **Styles ▸ Chart & Grid** from the flowsheet context menu.

7.5 THE EQUIPMENT GANTT CHART (EGC)

The equipment Gantt chart presents an overview of the entire schedule for a single or multiple batches as a Gantt chart from the equipment resources viewpoint. To display this chart for a single batch, select **Tasks ▸ Gantt Charts ▸ Equipment GC** and for multiple batches select **Tasks ▸ Gantt Charts ▸ Equipment GC (Multiple Batches)** from the main menu. For information on the Equipment Gantt chart see 6.2b Equipment Gantt Chart.

For more details on the EGC interfaces, see also:

- Equipment Gantt Chart (Single Batch)
- Equipment Gantt Chart (Multiple Batches)

7.6 THE EQUIPMENT OCCUPANCY CHART (EOC)

This chart displays information on equipment occupancy as a function of time for single or multiple batches and it enables the user to readily visualize the equipment time bottleneck. This chart comes up when you select **Charts ▸ Equipment Occupancy ▸ Single Batch** or **Charts ▸ Equipment Occupancy ▸ Multiple Batches** or if batch procedures in continuous process **Charts ▸ Equipment Occupancy ▸ Selected Time Horizon** from the main menu. For information on the Equipment Occupancy chart see 6.2a Equipment Occupancy Chart.

For more details on the EOC interfaces, see also:

- Equipment Occupancy Chart (Single Batch)
- Equipment Occupancy Chart (Multiple Batches)

8 PROCESS PROPERTIES & SIMULATION

Construction of a simulation model requires you to deal with several entities: pure components, stock mixtures, unit procedures, equipment resources, process streams, unit operations, heat transfer agents, labor types and so on. It is important to understand that all of the above are mere pieces of a large puzzle that is nothing other than the process itself, as an entity of its own. And just as each of the individual pieces has its own properties (think of all the properties that pure components or stock mixtures have) so does a process (as a whole). The properties of a process extend along several different dimensions: some affect the appearance of its elements (e.g. unit procedure icons and streams, see 8.3 Default Style for Process Elements); others affect the way the simulation calculations are carried out (e.g. identification of loops and tear streams, see 8.14g Loop Identification and Tear Stream Selection, or the convergence strategy and tolerance, see 8.14h Convergence Strategy); others affect how the economic calculations are carried out (e.g. expected lifetime for a process, what cost components should be included in the annual operating cost calculation, etc., see 9.2 Total Capital Investment); finally others are simulation results and as derivative quantities are not editable by the user (e.g. the minimum cycle time of the process, the maximum number of batches that can be executed per year, etc.). Most of the properties of the process as an entity of its own, are accessed from either the submenu under **Edit ▸ Process**

Options ▸ ... or from the flowsheet's command menu: that is the menu that appears when you right-click over an unoccupied area of the process drawing.

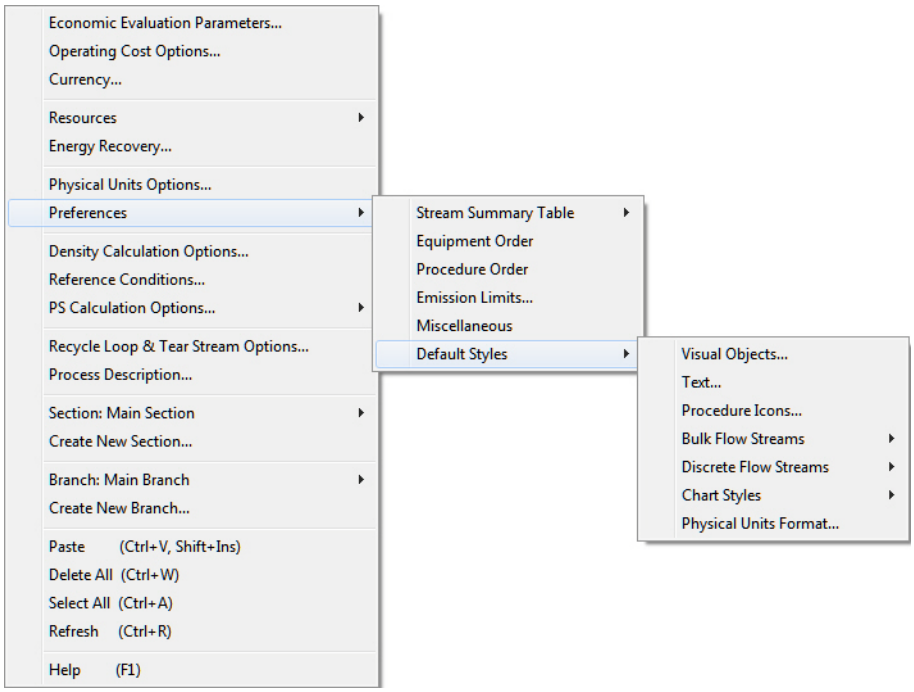


Figure 8.1: The command (context) menu for the process.

8.1 SECTIONS & BRANCHES

The concepts of process sections and branches exist to facilitate reporting of results for costing, economic evaluation, and resource requirements (materials, labor, power, heat transfer agents, etc.) of integrated large processes. A process section is simply a group of unit procedures that are put together with a certain goal in mind. For instance, typical sections in a process describing a biochemical plant might include the following:

1. Raw material preparation
2. Fermentation
3. Primary recovery
4. Product isolation
5. Final purification
6. Product formulation and packaging

A process branch is simply a sequence (in fixed order) of process sections that work towards a given goal. For instance, in a complicated, multi-step chemical synthesis process (quite common for synthetic pharmaceuticals and agrochemicals), you may want to distinguish

between the main path and the side-synthesis paths (frequently performed by toll manufacturers).

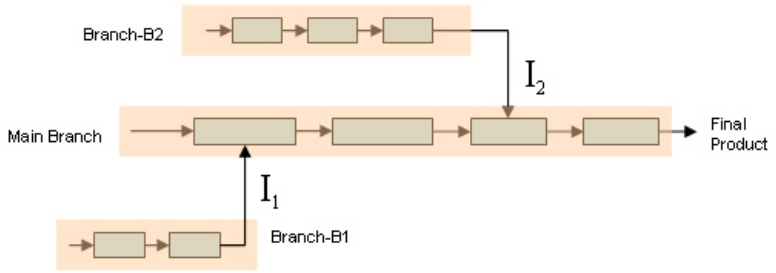
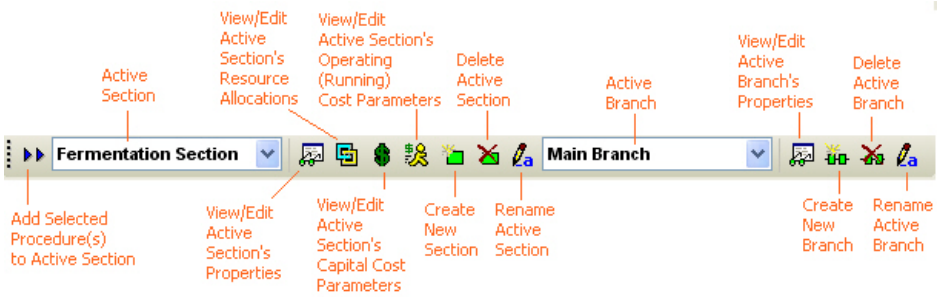


Figure 8.2: Breaking up a Large Process in Branches & Sections.

For the purposes of this application, branches don't serve currently any functional purpose other than dictating to the program how to report section results (branch-by- branch). By default each process is assumed to be made up of a single ('Main') branch and that main branch is assumed to contain a single ('Main') section. Even though you can add more sections to the 'Main' branch (and you can even rename the main branch to anything you wish) you cannot delete the branch that is designated as 'Main'. Similarly, you can add more sections to a branch and you can rename the 'main' section of a branch, but you cannot delete the section designated as the 'main' section of a branch. All parameters related to sections and branches of a process can be accessed from the Section <SectionName> and Branch <BranchName> submenus of the flowsheet's context menu or (as a shortcut) from buttons shown on the Sections & Branches Toolbar.

8.1a Sections & Branches Toolbar



You can create, delete and rename a section by clicking on the corresponding toolbar button. Similar buttons also exist for branches. If there are more than one sections (or branches) defined, then you can select from the drop-down controls the one you wish to be the 'active' section (or branch). By default the active branch is the 'Main Branch' and the active section is the 'Main Section'. Every time you add a unit procedure, it is automatically added to the active section.

8.1b Adding (Creating) a New Section

As mentioned elsewhere, each process file is automatically given a default branch (named 'Main Branch') that contains a single section (named 'Main Section'). Even though you can

rename the ‘main’ section (and the ‘main’ branch) to anything you like, you cannot delete it. If you have renamed the ‘main’ section, and have added several others, you can identify the section that still is recognized by the application as the ‘main’ section by visiting the Section Properties Dialog: Allocation tab.

▶ To add a new section...

1. Select the branch where the section will belong by selecting the active branch in the Section & Branches Toolbar.
2. Bring up the flowsheet’s context menu (by right-clicking on an unoccupied area of the flowsheet) and select **Create New Section**. As a shortcut, you can click on the button of the section toolbar.
3. In the ensuing dialog, type the name of the Section. Note that all section names in a branch must be unique. After you exit the dialog, the new section will have been added to the list of sections available to chose as the active section for the active branch. To verify that the new section has been created click on the drop-down of the listbox with all of the currently active branch’s section names, and you should see the new section that you just created.

A newly created section is added to the end of the branch’s queue and has no procedures in it. To add procedures to the section, see 8.1c Adding Unit Procedures to a Section. To properly place the section’s order in the sequence of all sections of the active branch, please visit the Branch Properties Dialog.

8.1c Adding Unit Procedures to a Section

When a new section is created it does not contain any procedures. You can add unit procedures to a section in two ways:

(a) You can add existing unit procedures that currently belong to a different section, see To add existing unit procedure(s) to a section..., or

(b) You can add new unit procedure that you will be creating next; simply select the desired section as the active section, and then create the unit procedures that you wish. They will automatically be added to the newly appointed active section.

▶ To add existing unit procedure(s) to a section...

1. Select the destination section as the active section from the section listbox of the toolbar. If the section you want is not listed, then make sure you select the branch that owns the section first.
2. Make sure you are in select mode (the button is pressed on the main toolbar). Select the unit procedure(s) you wish to move to the selected active section.
3. Click on the “Add to Section” button (first on the left on the section toolbar)

.

*The 'Add to Section' button may be inactive if either (a) you have not selected any procedure(s) or (b) the selected procedure(s) already belong to the active section. You can view which procedures belong to existing sections bring up the Procedure Utilization Breakdown interface (**View ▸ Utilization Breakdown ▸ Procedures**); to view which equipment resources belong to each section, bring up the Equipment Utilization Breakdown interface (**View ▸ Utilization Breakdown ▸ Equipment**).*

If desired, you can assign a special color for a section so that all icons for procedures that belong to that section show in a uniform color. A section can also be given a special naming and/or numbering scheme for each procedure, stream or equipment added by the user. For details on how to accomplish the above see Section Properties Dialog.

8.1d Section Properties

Each section maintains a large set of properties that relate to several aspects of its functionality. Some properties are related to its contribution to the economics (capital and/or operating cost) of the process (see Capital Investment Dialog and Operating Cost Adjustments Dialog); others may be related to its resource utilization (see Section Resource Allocation Dialog). Some of these properties are described below. Then there's another whole set of general properties that relate to the appearance of the procedure icons that belong to the section or to an optional definition of yields around a section or to its possible allocation to a database site, etc. You can access and modify the section's general properties from the Section Properties Dialog.

▶ **To edit a section's general properties...**

1. Make sure the section is selected as the active section in the Sections & Branches Toolbar.
2. Bring up the flowsheet's command menu (by right-clicking on an unoccupied area of the flowsheet).
3. Select **Section <SectionName> ▸ Properties**
   (as a shortcut you can click on the on the **View/Edit** button ( ) of the sections and branches toolbar, the one displayed right next to the active section display).

COLOR OF UNIT PROCEDURE ICONS IN A SECTION

You can designate a special color to be used when displaying the icons of unit procedures assigned to a section (in order to be easily distinguished in a large flowsheet). This assignment is made from the Section Properties Dialog: Icon Color tab. If you later change your mind and wish to have the icons of the section simply follow the general (common) icon color used for all procedures in the flowsheet (as set in the process settings for icon style preference, see 8.3 Default Style for Process Elements) then revisit the Section Properties Dialog: Icon Color tab and select 'Use Default Color' this time.

STARTING MATERIAL, ACTIVE PRODUCT AND SECTION YIELDS

You can select from all the input streams to procedures that belong to a section, one stream as the main 'input' of the section representing the **starting material**. Similarly, you can select from all streams on procedures that exit the section, one as the designated 'output' of the section, representing the **active product**. Instead of using the entire stream as reference flow for the starting material you could, instead, pick just a single component in that stream. Also,

you can designate which other components represent **impurities**. If A is the mass flow of the active product, S is the mass flow of the starting material and X is the mass flow of impurities, (based on the selections made by the user), then the application will calculate the following yield indices around a section:

Gross Mass Yield: (Aout + Xout) / (Sin+Xin)

Refined Mass Yield: Aout / Sin

Molar Yield: Aout (in moles) / Sin (in moles)

All of the section's yield-related properties described above can be viewed and/or edited from the Section Properties Dialog: Yields tab.

SECTION ALLOCATION

Every section is associated with a (real or hypothetical) physical site whose equipment and resources are employed by the section's operations in order to carry out their tasks. A default **generic site** is assumed to exist behind any section that is created. The generic site is a hypothetical entity with no limits on the type of available resources (labor, heat transfer agents, etc.) or the type and size of available equipment. When a section is associated with the generic site it is said to be **non-allocated**. Any operation in a procedure owned by a non-allocated section has at its disposal essentially any type of resource that is included in the system and user database. For instance, when selecting a heat transfer agent from an operation's i/o simulation dialog, the corresponding drop-down presents all agents that are currently registered in the process as well as all agents that are currently found in the user's databank. For users who have taken the time to populate SuperPro Designer's site database (see 15.13 Sites & Resources Databank) there are more exiting options if a user decides to match a section to a database site. This association, called **allocation**, essentially implies that the user makes the commitment to execute all operations contained in that section within the confines of the database site (as it is capture in the user database). The allocation of a process section to a database site can be made from the Section Properties Dialog: Allocation tab. Once the link between a process section and a database site has been established, you can proceed to further allocate all the resources employed by the operations in the section to available resources in the database site. For example, for each equipment resource currently assigned to host a procedure in the section, you can pick a database equipment that will actually be used to carry out the procedure's operations. For each heat transfer agent employed by any operation in that process section (e.g. 'HP Steam', 'Cooling Water', etc.) you can assign an available database resource. The process of allocating resources from a process section to database resources available to the allocated database site can be done easily from the Section Resource Allocation Dialog that can be displayed by selecting **Section <SectionName> ▸ Resource Assignment** from the flowsheet's command menu, or by clicking on the **Allocate Resources** button ( ) of the section toolbar.

CAPITAL & OPERATING COST PARAMETERS

As described elsewhere (see 9.1 Overview) there are several parameters that determine how the application calculates the capital (investment) related quantities (Direct Fixed Capital or DFC, working capital, startup and validation cost, etc.). To view the investment-related parameters select **Section <SectionName> ▸ Capital Cost Adjustments** from the flowsheet's command menu, or by click on the **Capital Cost Adjustments** button ( ) of the section toolbar. There are also several parameters that determine how this section contributes to the

annual operating cost of the entire process. To view the running (operating) cost related parameters **Section <SectionName> ▸ Operating Cost Adjustments** from the flowsheet's command menu, or by click on the **Operating Cost Adjustments** button ( ) of the section toolbar.

AUTO-NUMBERING RULES IN A SECTION

The application employes a general rule for assigning names to newly created procedures, streams and equipment. For a description of those rules see 8.20h Automatic Name Generation. If you wish to have a differentset of rules (unique) that apply to the procedures, streams and equipment that are created while a section is set as 'active', then you can visit the Section Properties Dialog: Auto-Numbering tab. For instance, if you wish all procedures added in a section to have a number in a certain range, then you can specify the starting number to be an appropriate value that will make all subsequent assignments fall in your range of choice. Please note that you can't set the prefix (or core string) used for each procedure as this is chosen based on the procedure type (or equipment type) and not the section that it belongs.

SECTION DESCRIPTION

As it is customary in many other objects contained in a process, the application allows you to specify a long descriptive text that may accurately convey any comments or special information that needs to be kept around the section. This commentary can be set from the Section Properties Dialog: Description tab. Such information is very critical in documenting and/or archiving any design decisions taken when the process was put together and thus allowing others to view/share such details at a later time.

8.2 BRANCHES

Branches are mainly a sequence of sections. Since it is not always possible for the program to infer a logical sequence of one section following another, the user can specify explicitly an order. The order of sections kept by the branch is the main property of the branch and can be edited from the 8.22c Branch Properties Dialog. This order is obeyed in reports where itemization of costs, amounts, etc. is presented in a section-by-section basis. Every process is created with a single branch (named 'Main Branch') and must have at least one branch (tagged as 'Main') that cannot be deleted (but if needed it can be renamed). The sections and branches toolbar has a drop-down control that displays the currently selected branch (active branch). All sections created (as described in Adding (Creating) a New Section) are added to the active branch. Even though you cannot re-assign a section from one branch to another, you can effectively accomplish the same by deleting the current section, creating a new section in the destination branch and then adding the procedures of the old section (now belonging to the 'main' section) to the new section (see To add existing unit procedure(s) to a section...).

8.2a Adding (Creating) a New Branch

▶ **Add a new branch...**

1. Bring up the flowsheet's context menu (by right-clicking on an unoccupied area of the flowsheet) and select **Create New Branch.** As a shortcut, you can click on the **Create New Branch** button ( ) of the sections and branches toolbar.
2. In the ensuing dialog, type the name of the branch. Note that all branch names in a process must be unique. After you exit the dialog, the new branch will have been added to the list of branches available to chose as the active branch. To verify that the new branch has been created click on the drop-down that displays all available branches and you should see the new branch that you just created.

A newly created branch is added to the process but it starts with only one section in it named 'Main Section' and designated as 'main' (i.e., it cannot be deleted). In order to add more sections to a branch, see 8.2b Adding Sections to a Branch.

8.2b Adding Sections to a Branch

Select the branch you wish to add a section as the active branch (from the sections and branches toolbar) and then follow the instructions for adding (creating) a new section (see 8.1b Adding (Creating) a New Section). The section will be added at the end of the sequence of sections held by the branch. If you wish to modify the section's order, please visit the Branch Properties Dialog by selecting **Branch <BranchName> ▸ Properties** from the flowsheet's context menu select. As a shortcut you can select on the **View/Edit Properties** button ( ) on the sections and branches toolbar (the one shown right next to the active branch name).

8.2c Branch Properties

SECTION ORDER

The most important branch property currently held by a branch is the order of its contained sections. The order is obeyed when presenting section-by-section results in reports or interface diagrams. To add, remove or edit the order of sections in a branch, please visit the Branch Properties Dialog: Properties tab.

BRANCH DESCRIPTION

As it is customary in many other objects contained in a process, the application allows you to specify a long descriptive text that may accurately convey comments or special information that needs to be kept around the branch. This commentary can be set from the Branch Properties Dialog: Description tab.

8.3 DEFAULT STYLE FOR PROCESS ELEMENTS

Almost every visual element presented by the application (procedure icons, streams, text, labels, charts, etc.) has an appearance that can be customized to a great extend to match each

user's preference. Each element is characterized by its own visual attributes. For example, icons may be described by their color, appearance of name labels (tags); streams may be characterized by the color and thickness of their line, the appearance and contents of their information tags, etc.; text shown on the flowsheet may be characterized by its color, font choice, frame and/or fill-in pattern, etc. On the other hand, interface elements like time charts may be described by an altogether different set of choices: units for the time axis and the dependent variable displayed (power, material amount or rate, etc.), color of the chart lines, etc. The collection of all such visual attributes defines what we call the **visual style** (or **style** for short) for that type of element. Each process file maintains a long list of default styles for many of the elements presented at various interfaces. For example, there's a default visual style for drawing bulk streams, and every stream you draw (even though you don't explicitly request it at the time) utilizes that style to present itself on the workspace. The interface for accessing a specific element's style may be slightly different, but as a general guideline, look for an entry named **Edit Style** in their context menu. For example, if your bring up the context menu for a procedure icon (right-click over the icon) and select **Style ▸ Edit.** its visual style dialog will appear. The default styles can be edited by selecting an entry in the **Default Preferences** menu (part of the flowsheet's context menu) shown in Figure 8.3. All such defaults are kept as part of the specific process and will not apply to the next process file that may be started later:

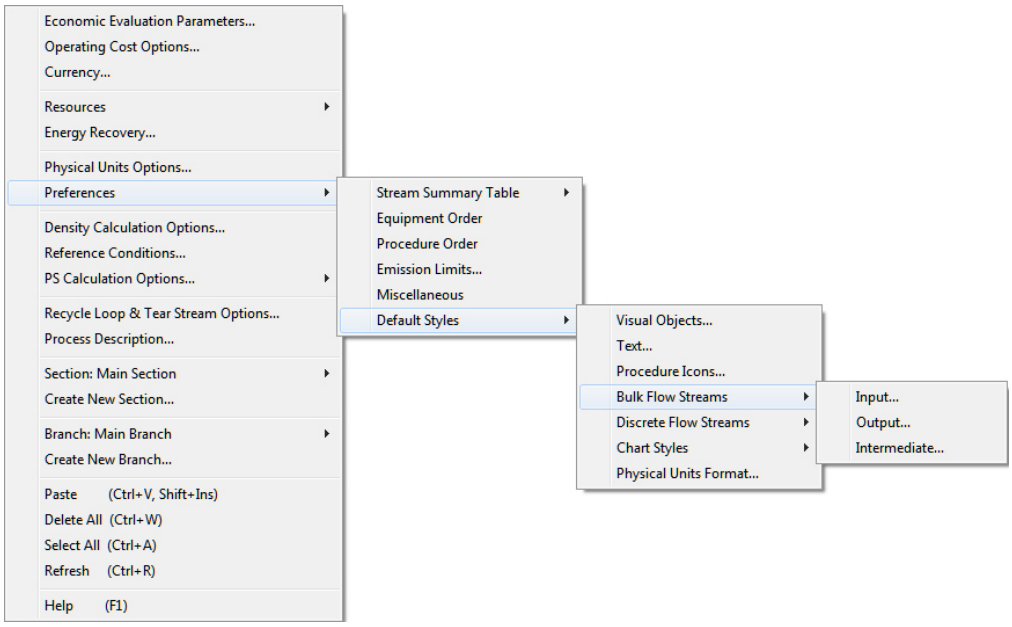


Figure 8.3: The 'Preferences' Menu Option for a Process.

Currently, a process file maintains default styles for the following item types:

Visual Objects	- Outline color, thickness, pattern. For interface, see Line Style Dialog.

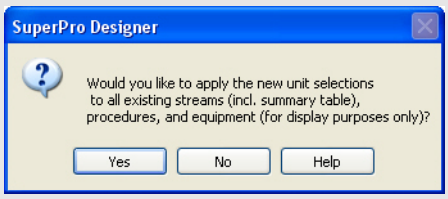
Text Objects	- Text: font, color. - Frame: outline color, thickness, pattern, shape, fill-in color For interface see Shape Style Dialog.
Procedure Icons	- Icon: Color, display (or not) of name, description tag, misc. indicators (multiple units, equipment sharing, etc.), equipment allocation signs, information tag. - Name, Description & Allocation Labels: Options for text (font, color) and frame (outline color, thickness, pattern, fill-in color). For interface see Unit Procedure Icon Style Dialog.
Bulk Flow Streams: Input, Output, Intermediate	- Stream line attributes (color, thickness, pattern) - Display (or hide) name tag and information tag - Name label properties (font choice, color, frame outline color, etc.) - Name label location (above, below or over horizontal / vertical segment). - Information tag properties (font choice, color, frame outline color etc.) - Information tag location (above, below or over horizontal / vertical segment). For interface see Stream Style Dialog.
Discrete Flow Streams: Input, Output, Intermediate	- Same as above, only for discrete flow streams. For interface see Stream Style Dialog.
Chart Styles	- Time Line, Graph Style Dialog (All Time Charts): Time Line Tab. - Gantt Charts (Operations, Equipment), Operations Gantt Chart Style Dialog and Equipment Gantt Chart Style Dialog. - Equipment Occupancy Chart, Equipment Occupancy Chart Style Dialog. - Power Demand & Generation Chart, Power Chart Style Dialog. - Utility Consumption / Inventory, Utility Chart Style Dialog. - Labor Demand, see Labor Chart Style Dialog. - Material Entering, Consumption/Inventory, Material Chart Style Dialog. - Material Exiting, Production/Inventory, Material Chart Style Dialog. - Storage Units (Demand/Deposit) see Storage Unit Supply (or Receive) Chart Style Dialog, and Storage Units (Demand/Deposit) Inventory, see Storage Unit Supply (or Receive) Inventory Chart Style Dialog. - Throughput Utilization Chart, Style for Throughput Utilization Chart Dialog. - Batch Potential Chart, Style for Throughput Potential Chart Dialog. - Auxiliary Equipment Demand Chart (for CIP skids CIP Skid Demand Chart Style Dialog, for SIP panels SIP Panel Demand Char Style Dialog - Equipment Occupancy Factors, Graph Style for Equipment Occupancy Data Chart.

Physical Quantities Format	Select Font, Color and Fill-in Color, Borders, Alignment and Format for a variety of physical quantities (such as Duration, Time Line, Total Mass, Liq/Sol Mass, Liq/Sol Density, Liq/Sol Volume, etc.) as they appear in Equipment Contents tables and Procedure Overview tables; see Physical Quantities Format Dialog.

8.4 UNITS OF MEASURE (PHYSICAL UNITS OPTIONS)

By default, the software always uses the International System of Units of Measure (SI Units) for all of the quantities displayed (mass, temperature, pressure, volume, densities, flowrates, etc.). Even if one wanted to stay within this system of units, it may be convenient to use one choice for stream flows (e.g.'L/min') but another for heat transfer agent flows (e.g. 'm^3/h'). The application offers the Physical Units Options Dialog that allows you to tweak the default choices used in certain contexts. This dialog can be viewed when selecting **Edit ▸ Process Options ▸ Physical Units Options** from the application's main menu or as a shortcut, **Physical Units Options** from the flowsheet's command menu. From the dialog you can choose any apply one of three buttons that make a consistent set of choices for all quantities: one applies all fundamental SI units, the other applies all fundamental British units and the third (labeled 'Preset Defaults') chooses units within (or derived from) the SI system of units. Of course, users can always overwrite the default choices in places of their liking. For example,

When exiting the physical units choice dialog by clicking on the OK button, the application will bring up the following question If you answer 'Yes' then any previous settings and/or


SuperPro Designer
Would you like to apply the new unit selections to all existing streams (incl. summary table), procedures, and equipment (for display purposes only)?
Yes
No
Help

overwrites that were specified in streams, operations, equipment, etc. will be lost and all displays of quantities will follow the unit choices as set by this dialog. If you answer 'No' then the new setting will only e used for any streams, operations, equipment, etc. that may be created in the future, and any previously set choices will be kept as-is.

even though the default choice for viewing volumetric flows in streams may be 'L', you can change the setting on a particular stream dialog to be 'gal' or anything else.

8.5 PROCESS DOCUMENTATION (DESCRIPTION)

Besides the drawing of a process, it is often required to maintain other information about it that may be required to be kept in the lifetime or evolution of the process. The application allows you to keep some of that information about the process itself (just like it allows you to keep commentary about specific procedures, equipment resources, operations, etc.). The process-

related comments can be set from the Process Description Dialog. This dialog appears when selecting **Edit ▸ Process Options ▸ Process Description** from the application's main menu or by selecting **Process Description** from the flowsheet's context menu. The dialog that appears, allows you to set several fields with names (Company/Client, project name, plant location, revision number, etc.) as well as dates (approval date) and extensive commentary on the process that may be important to preserve for future (or other) viewers.

Besides keeping comments about the entire process (as part of the Process Description dialog) you can also keep comments around every object involved in the process: unit procedures, operations, streams, components, mixtures, equipment resources, sections, etc. When viewing the properties of any of the above objects, look for a tab labelled 'Comments'. You may type any text that you wish to be kept for archiving/documentation purposes in association with any of the above objects.

8.6 PROCEDURE & EQUIPMENT ORDER

8.6a Procedure Order

When the application needs to present a chart or a tree that includes the list of procedures, it chooses to display the procedures in an order that is the same consistent everywhere it appears. That is why the order of appearance of procedures in the Operations Gantt Chart (**Tasks ▸ Gantt Charts ▸ Operation GC**) or in the Utilization Breakdown tree (**View ▸ Utilization Breakdown ▸ Procedures**) or in the Throughput Analysis Utilization Factors chart (**Charts ▸ Throughput Analysis ▸ Utilization Factors**) is the same. This order is kept by the process object, and it can be either modified from any of the style dialogs of the interfaces that use it, or from the Include / Exclude / Order Unit Procedures Dialog that is accessible from the flowsheet's context menu (**Preferences ▸ Procedure Order**). You may chose to keep the order of procedures based on:

1. First time of engagement
2. Alphabetically (ascending)
3. Alphabetically (descending)
4. User's custom order

If you chose 1 - 3 above any new procedure added later is automatically included in the order based on the selected criterion. If you chose (4) above (Custom Order), any new procedure created after the order has been set, it is added to the end of the list.

8.6b Equipment Order

When the application needs to present a chart or a tree that includes the list of equipment resources, it chooses to display the equipment in an order that is the consistent everywhere it appears. That is why the order of appearance of equipment resources in the Equipment Gantt Chart (**Tasks ▸ Gantt Charts ▸ Equipment GC**) or in the Equipment Occupancy Chart (**Charts ▸ Equipment Occupancy ▸ Single (or Multiple)**) or in the Utilization Breakdown tree (**View ▸ Utilization Breakdown ▸ Equipment**) or in the Main Equipment Occupancy Data Table or Chart (**View ▸ Main Equipment Occupancy Data ▸ Chart** or **Table**) is the same. This order is kept by the process object, and it can be either modified from

any of the style dialogs of the interfaces that use it, or from the Include / Exclude / Order Equipment Dialog that is accessible from the flowsheet's context menu (**Preferences ▸ Equipment Order**). You may chose to keep the order of equipment resources based on:

1. First time of engagement
2. Alphabetically (ascending)
3. Alphabetically (descending)
4. User's custom order

If you chose 1 - 3 above, any new equipment resource is added (later), it is automatically included in the order based on the selected criterion. If you chose 'Custom Order', any new equipment created after the order has been set, it is added to the end of the list.

8.7 DRAWING SIZE

When adding unit procedures to a process, you have available a limited drawing space. The application perceives drawing space as the equivalent of an array of tiles (paper sheets) (H x V) where H is the number sheets of papers horizontally and V is the number of paper sheets vertically. By default, each process file is assumed to have available the equivalent pixel space of a 2x2 array of sheets in portrait mode. If the entire space is not directly visible to your screen (due to its resolution and/or size) then you can scroll horizontally and vertically to see the ends of the drawing space. Of course if needed, you can change according to your needs, the drawing size for your flowsheet. Select **File ▸ Drawing Size** from the application's main menu and you will be presented with a dialog that allows you to change the number of sheets that dictate the space available across or vertically as well as the paper's orientation (landscape vs. portrait). If more than one printers are available to you (locally or via your LAN) you can use this dialog to pick a printer of choice.

When selecting the size of the drawing area based on a non-standard paper size and the file is later opened up on the same PC (or a different PC) at a time when that paper is NOT selected as the default paper size, the application will re-paginate the document's drawing size and recalculate the number of horizontal and vertical pages needed to provide sufficient drawing space based on the currently selected default paper. This may result in undesired relocation of icons on different pages.

SCREEN RESOLUTION

When adding elements to a flowsheet (unit procedures, streams, text labels or any other visual enhancements) their appearance (size and location) depends on the current screen resolution. If you save a flowsheet in a given resolution (e.g. 1280x1024) and later open the flowsheet on the same (or different) PC when the active resolution is something other than 1280x1024 you will notice some changes. The icon images of the unit procedures may appear larger (if the new resolution is smaller than 1280x1024) or smaller (if the new resolution is higher than 1280x1024). Also, the icons will appear to be either squeezed together (if the new resolution is smaller than 1280x1024) or spread apart (if the new resolution is higher than 1280x1024). To

avoid such unexpected appearance on the flowsheet you should try to use the same resolution for saving the file as when you will be presenting to others.

If you must chance the possibility that others may open your files in a resolution other than your, then to minimize the effects of resolution change, it is recommended that you arrange your icons and save the file in the lowest possible resolution that may be used by the file viewers. This way, if the file is opened at a higher resolution, the icons may be more spread apart (and possible fall on different pages) but at least they will still be comfortably viewable on a computer presentation.

8.8 OVERVIEW NAVIGATOR

When drawing a rather large process, it is very easy to require multiple pages of drawing space horizontally and vertically. Scrolling using the scroll bars will change the window of view. However, sometimes it becomes very tedious to have to scroll several times until you locate the area of the process that you want to bring to focus. Furthermore, it is very easy to be lost when only viewing a limited amount of the process flowsheet. For users who may have to explore such large flowsheets, the Overview Navigator will be an invaluable tool to have at your

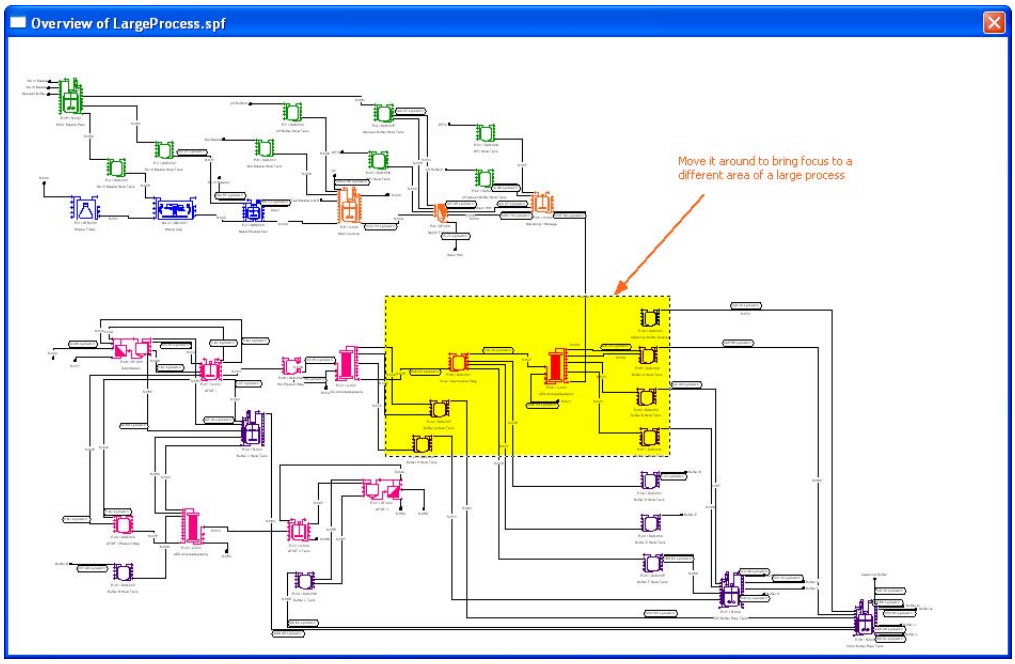


Figure 8.4: The overview navigator.

disposal. Selecting **View ▸ Overview Navigator** from the application's main menu, or clicking on the **Toggle Overview Navigator** button ( ) of the main toolbar will bring up a window that presents (in a zoomed out mode) the following:

(a) The entire process drawing

(b) The area of the process currently viewable by your workspace.

You can grab (click-and-drag) the viewable area around the process to change the focus in your workspace. When you have moved the focus to the area you would like to work with, you can close the navigator window and return to your main interface.

8.9 SEARCH AND LOCATE PROCESS ELEMENTS

When dealing with a large process flowsheet, it is sometimes difficult (or time consuming) to locate a specific element (unit procedure, equipment, stream or operation). The Find Dialog can help locate what you want in a flash. To activate the search interface simply type **Ctrl+F** (or select from the application's main menu). The following dialog appears:

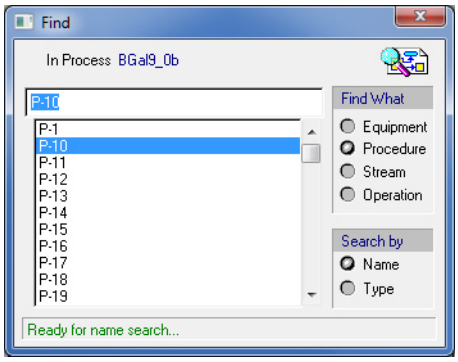


Figure 8.5: The Search & Locate (Find) Dialog.

Notice that the dialog will stay on top of every other open workspace and stay wherever it may be convenient for you. Also notice that the focus of search can only be one process at a time. Therefore, even if you have multiple files open at the same time, only the process that is currently active will be searched.

You may search for a given main equipment resource, unit procedure, stream or operation by either its name or its type. For example, you may want to find out all the 'Charge' operations in a process. Select 'Search by Type' and then from the listbox, pick 'Charge' and click on the **Find** button ( ), or simply double-click on the listbox entry. Notice that the application will scroll and select (show in red) a unit procedure where a 'Charge' operation is included. If you click again on the find button, then the next unit procedure where the search criteria matches will be located and shown as selected.

When you are searching by name, first pick the type of process element you are searching for (e.g. procedure) and then start typing in the edit box the name of the element. Notice that as you type more characters, the application scrolls down to the next possible match. If the string of characters no longer matches any of the available choices, the 'Find' dialog will display at the bottom a message indicating that 'No matches can be found'.

8.10 PROCESS EXPLORER

Building a process engages several objects (elements) either directly or indirectly: main equipment resources, auxiliary equipment (CIP skids, transfer lines, etc.), materials (pure components and stock mixtures, heat transfer agents, etc.). For each type of those objects, the application has a dedicated interface that lists all members and allows the editing of their properties. For example, you can visit the Pure Component Registration Dialog and see a list of all the pure components currently engaged in a process. Similarly, you can see all the heat transfer agents involved in the entire process by selecting **View ▸ Overview Navigator** and viewing the List of Heat Transfer Agents Currently in Use. All such interfaces exist but they are spread around under different menus. Starting with version 8.0, we have introduced the Process Explorer interface that makes viewing and accessing all those elements much easier.

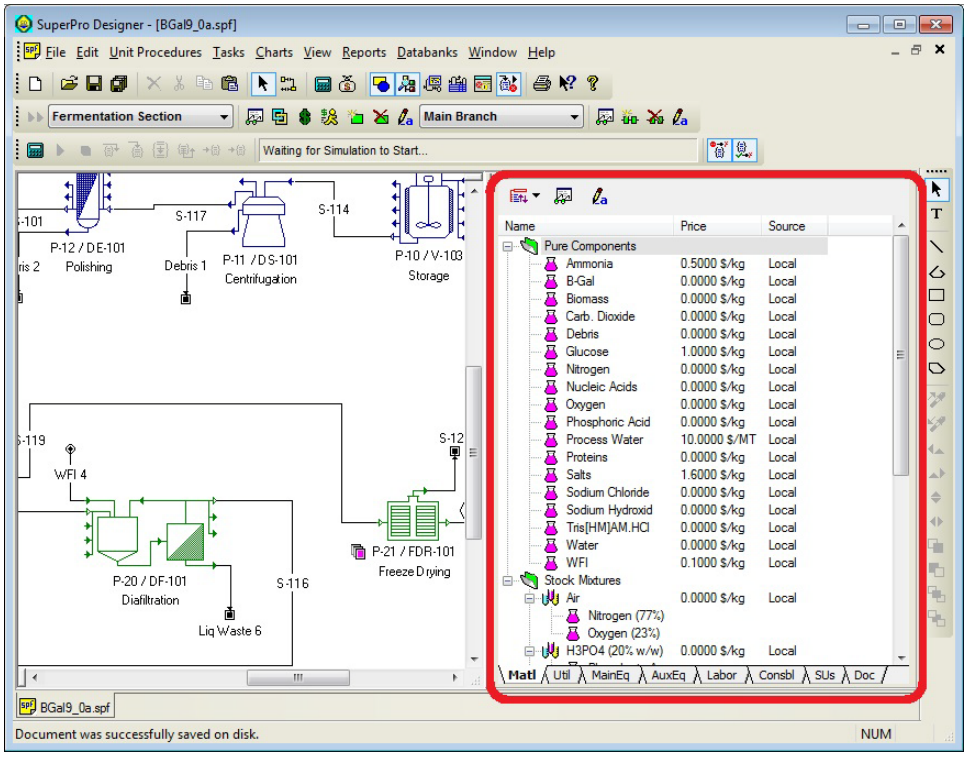


Figure 8.6: The process explorer interface.

If you click on the **Toggle Process Explorer** button ( ) of the main toolbar (or select **View ▸ Process Explorer** from the main menu), a multi-tabbed toolbar will appear (see area

circled in red in Figure 8.6). You may also show or hide this toolbar by right-clicking over any of the visible toolbars, in which case a list of all available toolbars will appear:

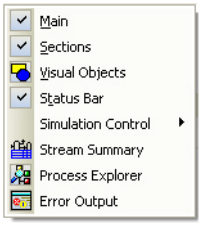


Figure 8.7: Toolbar Show/Hide Menu.

You may then select **Process Explorer** to show (or hide) the process explorer toolbar.

This toolbar can be docked vertically either to the far right (default) or the far-left of the workspace, or it can be left floating (double-click on the title bar of the process explorer to turn the "floating" behavior on or off).

Notice that the toolbar has multiple tabs (shown at the bottom of the circled area in Figure 8.4 above). Selecting each tab will present a catalog of those items if any of them is included in the process. You can customize the number of tabs that you wish to appear here by right-clicking over the tab area to show/hide a particular tab. The Process Explorer tabs and their contents include:

Matl	All pure components and stock mixtures registered currently in the process. For each ingredient its purchase price is directly displayed as well as its source (database or local definition).
Util	All registered utilities: Heating Agents, Cooling Agents and Power Types.
MainEq	Main Equipment Resources: The equipment are grouped by category (Centrifuges, Chrom. Columns, Dryers, Filters, Reactors & Fermentors, Storage, etc.). For each entry, we display its size (and units) and the number of equipment units Nu (operating simultaneously), the number of staggered sets, Ns and the number of backup (standby) units, Nb
AuxEq	All auxiliary equipment resources. Currently the application supports only CIP skids and SIP panels.
Labor	All labor types involved in the operations contained in the process. For each labor type, we display the adjusted basic labor rate and the lumped rate.
Consbl	All consumables involved in all equipment resources that require them are listed in this tab. They are grouped by their type (membranes, resins, etc.). For each item, its price is also directly displayed.
SUs	Supply and receiving storage units. For each such unit, we display (as part of its name in parenthesis) either the name of the supplied material (for supply units) or the type of the waste (in case of receiving units); we also display the purchase (for supply units) or waste treatment (for receiving units) price.

Doc

All documentation embedded within the project model. This could include text boxes that have been added to the flowsheet, comments related to specific flowsheet branches or sections, or comments related to unit procedures, operations, or equipment units (specified by the user through Description or Comments tabs). The upper pane of the Doc tab displays the location of each documentation item (grouped by type). The lower pane of the Doc tab displays the contents of a given item after it has been selected in the upper pane.

8.11 THE STREAM SUMMARY TABLE

Oftentimes, it is desirable to focus our attention on certain streams and more specifically on certain properties of those streams. Perhaps the flowrate of a certain component in a stream may be very critical, or the mole fraction of a component in a stream may be of greatest importance amongst your simulation outputs. The stream summary table serves exactly that need. It is a customizable stream table summary that you can include the streams you wish and view only the stream properties that are important for your process. It is shown as a separate tab on the horizontal toolbar (sharing space with the error output window) shown (originally) at the bottom of the workspace (but it can be also be docked at the top of the workspace or be left floating). A sample stream summary table is shown below

Stream Summary Table (BGal7_5a)

Time Ref: Batch		Air	Nutrients	Ammonia	Product
Type			Raw Material	Raw Material	Revenue
Total Flow	kg	47313.4176	7169.0000	395.0000	89.5199
Temperature	°C	25.00	25.00	25.00	12.00
Pressure	bar	1.013	1.013	1.013	1.013
Total Contents	kg	47313.4176	7169.0000	395.0000	89.5199
Ammonia		0.0000	0.0000	395.0000	0.0000
B-Gal		0.0000	0.0000	0.0000	85.7153
Biomass		0.0000	0.0000	0.0000	0.0000
Carb. Dioxide		0.0000	0.0000	0.0000	0.0000
Debris		0.0000	0.0000	0.0000	0.0000
Glucose		0.0000	6143.0000	0.0000	0.0000
Nitrogen		36294.9684	0.0000	0.0000	0.0000
Nucleic Acids		0.0000	0.0000	0.0000	0.0000
Oxygen		11018.4492	0.0000	0.0000	0.0000
Phosphoric Acid		0.0000	0.0000	0.0000	0.0000
Process Water		0.0000	0.0000	0.0000	0.0000
Proteins		0.0000	0.0000	0.0000	0.0003
Salts		0.0000	1026.0000	0.0000	0.0000
Sodium Chloride		0.0000	0.0000	0.0000	0.0298
Sodium Hydroxid		0.0000	0.0000	0.0000	0.0000
Tris(HM1AM.HCl		0.0000	0.0000	0.0000	0.0000

StreamSummary

Figure 8.8: The Stream Summary Table.

You can show/hide the stream summary table by selecting **View ▸ Stream Summary Table** from the application's main menu, or by clicking on the **Toggle Stream Summary Table** button ( ) of the main toolbar. The table when first viewed is empty (has nothing to show). To display your choice of stream properties for a set of streams that may be of importance to you, right-click over the table (to display the stream summary table's context menu) and from the menu select **Edit Contents**.

STREAM TABLE MENU OF OPERATIONS (CONTEXT MENU)

If you right-click over the stream table, the following menu will appear:

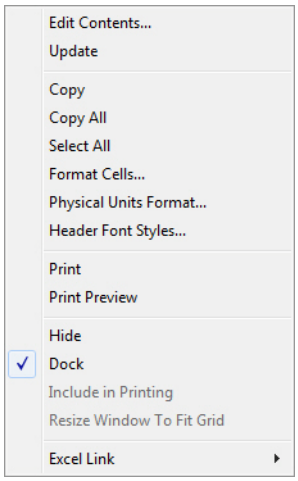


Figure 8.9: The Stream Summary Table's Context (Right-Click) Menu.

From this menu you may dictate that the table be floating or docked (check or un-check **Dock**). If the table is floating then you resized it and locate it any where you wish over the flowsheet. In fact, you can pick **Include in Printing** and then print the flowsheet; this way the flowsheet will come out with the stream table showing on top. You can directly **Print** (or **Print Preview**) the table alone. When the table is floating (thus re-sizable) you can select **Resize Window to Fit Grid** to make sure the window is sized just right to fit the contents of the grid (if that's possible). You may copy either a selected range of cells or all the stream's contents by selecting **Copy** or **Copy All** and then paste them in another application. Keep in mind that the stream table contents change from time to time: for example, after performing a M&E balance calculation, some of the flows, compositions, etc. for streams shown on the table may change. The application will updated the table's contents automatically. If you are monitoring an input stream, the values may change if you visit the i/o dialog of the input stream and change some of its properties. The stream table contents, once again, should change to reflect the new values. If you believe that any part of the table is still not up-to-date, you can issue an **Update** command to force the refreshing of the table's contents.

CUSTOMIZING THE STREAM TABLE CONTENTS

Selecting **Edit Contents** from the table's context menu (see Figure 8.9) will present the Stream Summary Table: Edit Contents Dialog that allows you to customize the contents (rows and columns) of the table by specifying:

(a) Which streams to include: Streams can be process inputs, outputs or intermediates.

(b) Which stream properties to display for each stream: you can select from a long list of attributes which ones to include for monitoring directly on the table: stream classification, total flow, temperature, pressure, liquid/solid (L/S) flow, L/S volume, L/S density, total or specific enthalpies, heat capacity.

(c) Which component to skip from the total contents section, the liquid/solid section or the gaseous section (if needed).

FORMATTING A RANGE OF CELLS

If you highlight (select) a range of cells in the table and then select **Format Cells** from the table's context menu you will be presented with the Cell Format Dialog, that allows you to apply some visual formatting on the cells. Please note that the formatting will not be lost if:

(a) You edit the stream table's contents, or

(b) You close the process document

If you want to have some formatting be more of a permanent nature, then you should visit the Physical Quantities Format Dialog. Styles of row and column headers can be formatted by selecting **Header Font Styles...** from the tables context menu.

LINKING THE STREAM TABLE TO AN EXCEL SPREADSHEET

Sometimes you may find it necessary to have the contents of the table mapped into an Excel spreadsheet so that you can either show the values as part of an elaborate and highly customized report or simply feed the values to some other custom calculations captured as macros or scripts in the Excel file. For such cases, you will find the **Excel Link** feature extremely useful. Selecting **Excel Link ▸ Edit** from the command menu of the table will present you with the Link Table to MS-Excel® Dialog that can capture all the information needed so that the application can map all the values of the table straight into an Excel file. There's several options as to how exactly the updating will be done and they are all explained in detail in the documentation that is part of the dialog. Once a link has been established, the application will directly update the values of the displayed properties either after your command (selecting **Excel Link ▸ Update** from the command menu) or automatically (if the 'Auto-Update' feature is check in the Excel link specification).

The Excel Link information can also be customized by the COM interface of the application. Typically, users will specify all of the Excel Linking information using the application's interface (and save it as part of the process file) and later use the COM interface to update the Excel spreadsheet when convenient (e.g. after setting certain input variables and re-solving the M&E balances). This is a relatively quick and convenient way to use a base case design for performing sensitivity calculations and easily record the output in Excel tables.

When you no longer need the Excel linking information to be part of the saved properties of the table, simply select **Excel Link ▸ Delete** from he command menu of the table.

8.12 PHYSICAL STATE CALCULATION OPTIONS

SuperPro Designer determines the physical state (PS) of material (i.e., the distribution of components between the vapor and liquid/solid state) by one of its two embedded toolboxes namely, the Shortcut and the Rigorous PS calculation toolbox. The Shortcut PS toolbox, "infers" the physical state of components by employing component-specific Vapor/Liquid split criteria. On the other hand, the Rigorous PS toolbox offers a more realistic approach by employing formal thermodynamic VLE models that take into account the interaction between the various components in the mixture. Its application however, relies on the availability and

accuracy of the respective model parameters such as Antoine coefficients, critical parameters, binary interaction coefficients, activity model coefficients, etc.

By default, the application utilizes the Shortcut PS toolbox to determine the physical state of components, everywhere in a process file. There are, however, certain unit procedures(e.g. Flash, Rigorous Distillation, Thin Film Evaporation, Condensation, etc.) that require, by nature, the Rigorous PS toolbox in order to carry out the modeling calculations of their respective operations. In this case, the Shortcut toolbox is not applicable and the Rigorous toolbox is employed as the only option (see Rigorous Toolbox-Only Unit Procedures).

8.12a The Shortcut Physical State Calculation Toolbox

The Shortcut toolbox determines the physical state of material in streams or procedure states by applying one of the following V/L split criteria to each individual component:

1. *Normal Boiling Point*. If the normal boiling point temperature of a component is higher than the temperature of the stream (or procedure state), then the component is assumed to be completely in the liquid/solid phase (i.e., its vapor fraction percentage is equal to 0%). Otherwise, it is assumed to be completely in the vapor phase (i.e., its vapor fraction percentage is equal to 100%). Clearly, this criterion does not account for the effects of pressure and consequently, for mixtures at pressures different than atmospheric, the Vapor Pressure criterion should be used.
2. V*apor Pressure (Antoine)*. If the boiling point temperature of a component at the pressure of the stream (as calculated by Antoine's correlation) is higher than the stream's operating temperature, then the component is assumed to be completely in the liquid/solid phase (i.e., its vapor fraction percentage is equal to 0%). Otherwise, it is assumed to be completely in the vapor phase (i.e., its vapor fraction percentage is equal to 100%).
3. *Liquid/Solid Only.* The component is assumed to be completely in the liquid/solid phase (i.e., its vapor fraction percentage is equal to 0%) regardless of the temperature and pressure of the stream.
4. *Vapor Only.* The component is assumed to be completely in the vapor phase (i.e., its vapor fraction percentage is equal to 1%) regardless of the temperature and pressure of the stream.
5. *Set Vapor Fraction*. This criterion allows you to set directly the vapor fraction percentage of a component to a value between 0 and 100%. The component is assumed to be partly in the vapor phase by that specific fraction, regardless of the temperature and pressure of the stream.

In certain cases, a component with the Boiling Point or Vapor Pressure V/L split criterion may have a vapor fraction percentage between 0 and 100% (in other words, that component is distributed between the vapor and liquid/solid state). Typically, this happens when the calculation engine performs an energy balance where a given enthalpy must be 'preserved' by the resulting stream (e.g., as a result of a mixing operation). In this case, the only way for the enthalpy to be attained is by distributing that component's presence between the vapor and liquid/solid state.

8.12b The Rigorous Physical State Calculation Toolbox

The Rigorous toolbox determines the distribution of components in the vapor and liquid phase by using thermodynamic VLE models. In the current version of SuperPro Designer, the following VLE models are supported:

1. *Raoult's Law.* This model assumes and ideal vapor liquid phase and therefore, should be considered as a shortcut for quick and robust Rigorous VLE calculations. The application of Raoult's law presupposes the knowledge of Antoine coefficients for the calculation of the vapor pressure of the pure components.
2. *Hybrid Raoult's law/Custom vapor fraction model*. In case that Antoine coefficients are not available for certain components, the program offers the possibility to directly set the vapor fraction percentage for them, thereby creating a hybrid Raoult's law/custom vapor fraction model.

The option to specify the component vapor fraction percentage and override the calculation of their K-values by the VLE model, is only available with Raoult's Law.

3. *Modified Raoult's Law.* This model assumes an ideal vapor phase and a non-ideal liquid phase described by means of an activity coefficient model. Besides from the Antoine coefficients, this model requires the activity coefficient model parameters (i.e., either for the Wilson or the NRTL model) for the components present in the mixture. If these parameters are not provided, the model becomes identical to Raoult's Law.
4. *Equation of State (EOS) Models*. An EOS model assumes non-ideal behavior for both the vapor and for the liquid phase. While EOS models are widely used in mixtures of hydrocarbons and light gases at sub-critical temperatures, they have an inherent inability to accurately capture the behavior of the liquid phase in polar mixtures (e.g. aqueous solutions). The application of an EOS model requires the availability of values for critical parameters and optionally, binary interaction coefficients. In the absence of the latter, the accuracy of the model may be significantly reduced.
5. *Gamma-Phi Models*. Gamma-phi models use an EOS to describe the vapor phase and an activity coefficient model to describe the liquid phase of a mixture. They can be used with all types of mixtures (including polar mixtures) at sub-critical temperatures. While gamma-phi models are considered to be the most accurate, their use is often limited by the requirement for both EOS binary interaction parameters and activity coefficient model parameters.

SuperPro Designer offers the option to exclude one or more components from VLE calculations. Excluded components are treated as if they belong to a separate, independent liquid/solid phase: they do not affect the molar fractions of the components that participate in the VLE model and are only taken into account in energy balances.

For a more elaborate description of the underlying thermodynamic theory as well as the various features available in SuperPro Designer regarding the vapor-liquid modeling, you may want to refer to "Vapor-Liquid Equilibrium Modeling".

8.12c Customizing the Physical State Calculation Options

Each process file keeps a set of default options for the Shortcut and Rigorous PS calculation toolboxes. These process-level default options are enforced on all newly-created input streams

and procedures. You can differentiate from these default options by visiting the corresponding PS options dialogue and checking the Overwrite button. Notice that all changes made to the PS calculation options at the process level are automatically propagated to all input streams and procedures in the flowsheet unless the Overwrite option has been enabled for any of them.

In addition, each procedure in a process file has its own set of default options for the Shortcut and Rigorous toolbox *as well as a default selection regarding which one of the two toolboxes will be used* for the calculation of the physical state of material. These procedure-level default options together with the toolbox selection are imposed to all of its procedure states and output streams. Again, you can differentiate from these default settings by visiting the corresponding PS options dialogue of the procedure state or output stream and checking the Overwrite button. Finally, any change to the default procedure PS toolbox options and toolbox selection will be automatically propagated to all of the procedure states and associated output streams unless the Overwrite option has been enabled for any of them. The inheritance tree of the PS calculation options is illustrated in Figure 8.10.

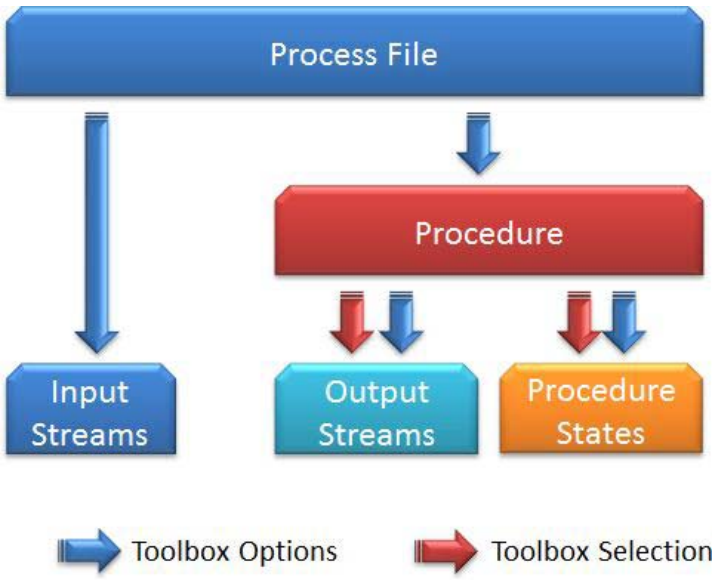


Figure 8.10: The inheritance tree of the physical state calculation options.

The option to assign a physical state calculation toolbox is only available for procedures, streams and procedure states (when exposed to the user). It is not available through the default settings held by the process file. In other words, a process file cannot assign a specific PS calculation toolbox to be used by all of its entities (i.e., streams, procedures and procedure states).

To customize the physical state calculation of material according to one's own needs, the user can either:

1. Change the default toolbox selection and toolbox options *at the process level*.
2. Change the default options for either one of the toolboxes *at the process level*.
3. Change the default toolbox selection and toolbox options and *at the procedure level*.

4. Customize/overwrite the toolbox options and toolbox selection *for specific streams and procedure states*.

CHANGING THE DEFAULT PS CALCULATION OPTIONS AT THE PROCESS LEVEL

Every new process file will, upon creation, use the Shortcut PS toolbox as the default selection for determining the physical state of material. To change the default toolbox selection at the process level, select **Edit ▸Process Options ▸PS Calculation Options▸Shortcut vs Rigorous**. Alternatively, you can right-click on anywhere in the flowsheet and select **PS Calculation Options▸Shortcut vs Rigorous.**

By default, the Shortcut PS toolbox infers the PS of material by employing the Normal Boiling Point V/L split criterion for all components. You can modify the process-level default V/L split criteria for each component by selecting the **Edit ▸Process Options ▸PS Calculation Options ▸Default Shortcut PS Calc. Toolbox** from the main menu or by bringing up the command (context) menu of the process (i.e., by right-clicking on anywhere in the flowsheet) and selecting **PS Calculation Options ▸Default Shortcut PS Calc. Toolbox.** For more details see: The Shortcut PS Calculation Toolbox Dialog.

The Rigorous PS calculation toolbox employs the Raoult's Law as its default VLE model. This option can be changed by selecting **Edit ▸Process Options ▸PS Calculation Options ▸Default Rigorous PS Calc. Toolbox** from the main menu or by presenting the context menu of the process (i.e., by right-clicking on anywhere in the flowsheet) and selecting **PS Calculation Options ▸Default Rigorous PS Calc. Toolbox.** For more details see: The Rigorous PS Calculation Toolbox Dialog.

CHANGING THE DEFAULT PS CALCULATION OPTIONS AT THE UNIT PROCEDURE LEVEL

To modify the default PS calculation options of a unit procedure, select the procedure by left-clicking on its icon and pick **Edit ▸Unit Procedure Options ▸Default PS Calc. Options** from the main menu. Alternatively, right-click on it to show its context menu and then select **Default PS Calc. Options.** In the Physical State Calc. Options dialog that appears, check the Overwrite button and proceed in making the desired modifications. For more information you are referred to 5.13 Procedure PS and Density Calculation Default Options.

TO CUSTOMIZE THE PS CALCULATION OPTIONS OF STREAMS

To change the PS calculation options of a stream, select the stream by left-clicking on it and pick **Edit ▸Stream Options ▸Simulation Data** or alternatively, double-click on it. In the dialog that appears, visit the Physical State tab, check the Overwrite option in the PS Calculation Options frame and proceed in making the desired modifications. For more information you are referred to 4.7d Stream Physical State Calculation Options.

TO CUSTOMIZE THE PS CALCULATION OPTIONS OF PROCEDURE STATES

To change the PS calculation options of a procedure state, select its associated unit procedure by left-clicking on it and pick **Edit ▸Unit Procedure Options▸Procedure State Options.** Alternatively, you can right-click on the associated unit procedure and select **Procedure State Options.** In the dialog that appears, visit the corresponding tab of the procedure state, check the Overwrite option in the PS Calculation Options frame and proceed in

making the desired modifications. For more information you are referred to 5.12a Procedure State Physical State Calculation Options.

In principle, the PS calculation options of streams only have an indirect impact on the simulation outputs through the calculation of their enthalpy content. In other words, the overall energy balance around a procedure will calculate the enthalpy content of input streams to that procedure based on the PS calculation options of these streams.

For procedure states on the other hand, the PS calculation options have a profound effect on simulation results. In design mode, the application calculates the size and the number of equipment units needed to accommodate the process requirements based on the liquid volume determined by the PS calculation options of the procedure state. In rating mode (i.e., when the size and number of units is given) the available liquid capacity is used as an upper limit constraint as to how much material can be processed per batch.

8.13 DENSITY CALCULATION OPTIONS

SuperPro Designer offers a set of customizable options for the calculation of the liquid and vapor density.

8.13a Liquid/Solid Phase Density Calculation Options

The program offers the following two options for the calculation of the liquid/solid phase density:

- the ideal mixture model, the density of the liquid phase, ρ_L, is calculated by the ratio of the total volume to the total mass:

$$\rho_L = \frac{m_L}{V_L} \qquad \text{eq. (8.1)}$$

where m_L

$$m_L = \sum_i m_i \qquad \text{eq. (8.2)}$$

$$V_L = \sum \lambda_i \frac{m_i}{\rho_i} \qquad \text{eq. (8.3)}$$

In eq. (8.3) above, m_i is the mass flowrate of the component *i* and λ_i are weight factors called *Volumetric Contribution Coefficients* (VCCs). It is possible to shift the calculated liquid density values to reflect ones needs by appropriate adjustment of the VCCs. In general, the following guidelines should be applied:

1. Full volume additivity (i.e., λ_i=1) leads to an overestimation of the volumetric flowrate and consequently, of the equipment size.
2. Values of λ_i lower than unity will reduce the contribution of component *i* to the overall liquid volumetric flowrate.
3. For solid components that fully dissolve into a solvent mixture, λ_i should be equal to zero.
4. For solid components that form a slurry with the solvent, λ_i should be equal to 0.2-0.3.

- ***User-Defined Density Value***

When this option is selected, the density of the liquid phase is set to a fixed value, regardless its composition and the operating conditions.

Liquid density calculation options also affect the volumetric flow of streams and procedure states.

8.13b Vapor Phase Density Calculation Options

The program offers the following options for the calculation of the vapor phase density:

- ***Ideal Gas Model.*** The density (molar volume) of the vapor phase is calculated under the assumption of the ideal gas law:

$$\rho_V = \frac{P}{RT} \qquad \text{eq. (8.4)}$$

User-Defined Density Value.The density of the vapor phase is set to a fixed value, regardless its composition and the operating conditions.

Modifying the density calculation options for the vapor phase impacts the volumetric flowrate of streams and procedure states but <u>not</u> the calculated equipment size.

OVERALL DENSITY OF TWO-PHASE STREAMS AND PROCEDURE STATES

In the case that material in a stream or procedure state exists in two phases, an overall (mixed) stream density is calculated by the following equation:

$$\rho_{mixed} = \frac{m_{mixed}}{V_{mixed}} = \frac{m_L + m_V}{V_L + V_V} = \frac{m_L + m_V}{\frac{m_L}{\rho_L} + \frac{m_V}{\rho_V}} \qquad \text{eq. (8.5)}$$

where m_L, V_L, ρ_L and m_V, V_V, ρ_V are the mass flowrate, the volumetric flowrate and density of the liquid and vapor phase, respectively.

8.13c Customizing the Density Calculation Options

Each process file keeps a set of default options for the calculation of the vapor and liquid/solid phase density. These options are automatically propagated to all of the streams and procedure states unless the Overwrite option has been enabled for any of them. You can shift the density values to more realistic bound by:

1. Changing the density calculation options *at the process level* or,
2. Overwriting the density calculation options *for specific streams and/or procedure states.*

In the current version of SuperPro, you do not have the option to modify the density calculation options at the unit procedure level.

CHANGING THE DEFAULT DENSITY CALCULATION OPTIONS AT THE PROCESS LEVEL

To set your own process-level preferences for the calculation of density, select **Edit ▸Process Options ▸Density Calculation Options** from the main menu or by selecting **Density Calculation Options** from the command menu of the process file. See also The Density Calculation Options Dialog.

CUSTOMIZING THE DENSITY CALCULATION OPTIONS OF STREAMS

To change the density calculation options of a stream, select the stream by left-clicking on it and pick **Edit ▸Stream Options ▸Simulation Data** or alternatively, double-click on it. In the dialog that appears, visit the Physical State tab, check the Overwrite options of either the liquid/solid or the vapor phase density and proceed in making the desired modifications. For more information see 4.7e Stream Density Calculation Options.

CUSTOMIZING THE DENSITY CALCULATION OPTIONS OF PROCEDURE STATES

To change the physical state calculation options of a procedure state, select its associated unit procedure by left-clicking on it and pick **Edit ▸Unit Procedure Options▸Procedure State Options.** Alternatively, you can right-click on the associated unit procedure and select **Procedure State Options.** In the dialog that appears, visit the corresponding procedure state tab, check the Overwrite option of either the liquid/solid or the vapor phase density and proceed in making the desired modifications. For more information see 5.12b Procedure State Density Calculation Options.

8.14 THE PROCESS SIMULATION ENGINE

8.14a Simulation 101

If you are new to process simulation, no need to worry. After several years of refinement, you will find that SuperPro Designer's interface takes away all the difficulty and intimidation for the novice user, yet after you go beyond the surface, you will find plenty of tools needed by seasoned simulation veterans in order to capture complex process interactions and generate accurate simulation results.

Putting together a batch process simulation is not unlike the task undertaken by a theatrical director with the goal of producing a stage performance in a theater. Even though, in principle, there are infinite details that can be attended to, there is only so much that the director can manage. Needless to say, that he or she cannot hope to have a successful production unless the important issues are dealt with.

'The Actors': Before you start thinking about any other aspect of the process simulation, it is wise to start thinking about the materials that will participate (the cast members). Such materials can be introduced in the form of either pure components or mixtures. It is materials that show up everywhere in the process: the make up the input streams that feed the process; they move from place to place, appearing inside equipment (as contents) and making things happen (reactions, separations, etc.). Finally, it is materials that need to show up at the right place (on the product streams) at the end of the process if everything went well.

'The Script': Every one on the stage needs to move around according to a script. Otherwise, nothing makes sense. In the same spirit, the backbone of a process is its expression as a sequence of actions (or scenes in the language of theater) that work towards producing the desired result. Each scene (unit procedure) along the way accomplishes a small task and sets up the stage for the next scene. Within each scene, there may be several acts one following another. In the simulation language of SuperPro Designer, those individual acts are represented by unit operations. Each act is timely set up to follow another until the scene is complete.

'The Stage Props': There are many items that need to be engaged during the performance: stage area, lights, microphones, costumes and other miscellaneous props used by the actors, etc. In the same manner, there are many resources that need to be engaged by the 'actors' (materials) as the recipe is executed: equipment needs to be available for hosting the individual steps; heating and/or cooling agents need to be engaged (at appropriate times and at a specified levels) to accomplish various heating/cooling tasks; CIP skids may be needed to engage in special vessel cleaning; labor (general or special) may be needed to supervise the execution of each action. Calculating the amount of resources needed to carry out the entire recipe and making sure that there are no sharing violations for items such as equipment etc. or upper limit violations for items such as labor availability etc. is clearly very important. It is your job, as the director, to time the events in the production such as none of the above unfortunate situations appear. In the language of SuperPro Designer, you get to decide the timing of all the operations, and the application in return will calculate the amount of resources needed at each step and will notify you if any such resource constraints are recorded.

8.14b Simplicity and the Art of Simulation

The objective of every simulation exercise is to build a model (using an appropriate software tool) that will capture the behavioral characteristics of an actual process so that it can be studied and evaluated with respect to any number of possible goals (design scope). If a new process facility is to be built, then the goal is typically economics. If the process is currently running on an existing facility, then the goal could be to increase the throughput and to identify possible bottlenecks; it could also be to assess the environmental impact and to propose modifications that may reduce the hazardous impact on the environment. Whatever the scope may be, it is very important that it is understood before undertaking the simulation project and always kept in mind as you make decisions on how to model the process. The user must understand that simulation modeling will never capture all the aspects of the real process in their fullest detail. It very difficult (practically impossible) to reproduce the innumerable aspects of a functional processing facility using computer models. There are so many intricacies in the way so many different parameters affect the performance of each unit operation. Furthermore, each one effect will demonstrate itself differently to the final product as it is propagated through the network of all other steps till the final product is delivered. However, do not allow the enormity of as ambitious a goal as to capture perfectly the workings of a real process intimidate you. Not only do we not need to capture all the aspects of a processing facility, but we should actually strive to leave out as many details as possible to the extend that they do not affect the behavioral aspects that are of interest. The greatest Renaissance master and one of the brightest engineering minds that ever lived, Leonardo da Vinci said: “Simplicity is the ultimate sophistication”. You do not need to include more and more in your model to make it be more sophisticated. You just need to include the parts that make it respond properly when it comes to measuring the outputs that are of importance to your particular study. Of course it requires a lot of experience and engineering knowledge to know what it is that you need to capture and what it is that you are allowed to leave out. Of course, it also requires that you keep in mind the scope of this exercise. “Make everything as simple as possible, but not simpler.” The previous quote attributed to A. Einstein captures very succinctly the essence of modeling. Leave out all those details that don’t matter. But make sure not to leave out the aspects that can make a difference.

8.14c Simulation Philosophy

Back in the early ‘80s, the first process simulation tools were developed to capture the complexities of purely continuous processes (such as the transformations that you encounter in a typical refinery plant). The representation of such processes is much simpler: the designer draws a flowsheet based on the material allocation (movement) from one piece of equipment to another. The final picture uniquely describes the process. There’s no material ‘hidden’ inside any of the equipment that needs to be accounted for in the material and energy balances. In other words, there are no equipment contents that need to be accounted for; only flows of material in and out of processing steps. All flows are kept in amounts per time (e.g. kg/h).

In a batch simulation, the time dimension (which is completely missing in a continuous simulation project) adds a new, very significant twist in the representation of the process. Each equipment is not necessarily used in a dedicated way to perform a single step during the process. Instead, as it is very often common, processing equipment host more than one steps: some during the early phase of a batch, some during later stages of the same batch (or even later batches.) A simple material allocation based on the process equipment and their in- and out-

flows of material would be very inadequate, as streams would be leaving and entering a process equipment several times, but the material they carried came (or left) at different times rendering this picture very confusing and misleading. Some other batch simulation tools, have adopted the time dimension as the principal guide to represent the process, and expect the designer to express the process in a 'recipe-execution'-like format:

1. Start by Charging 10L of material A into Vessel 101 (45 min)
2. Then, Charge 5L of material B into Vessel 101 (20 min)
3. Stir contents of Vessel 101 for 30 min.

...and so on.

Even though it is possible to accurately describe the entire recipe in a manner like the above, for a complex process, it becomes very cumbersome. Furthermore, there is no overall pictorial view that gives a viewer of this model an understanding of what is happening in the process. Another approach to batch simulation modeling requires the representation of each action as a dynamic and/or discrete set of equations. Such an approach, even though very be very useful for representing single operations it is hopelessly complex when applied to real-life processes. Furthermore, such an approach cannot integrate continuous steps as part of the process representation see Batch vs. Continuous Procedures.

OUR APPROACH TO BATCH PROCESS SIMULATION

The approach that was adopted by SuperPro Designer when it was originally conceived (in early 90s) is similar to what was eventually adopted and later (1997) became part of the ANSI/ISA-88 standard (or S-88 standard for short) for accurately addressing the needs of batch process control. According to the S-88 standard a process model (or process) consists of an ordered set of process stages; each process stage consists of an ordered set of process operations which in turn, is implemented as an ordered set of process actions. Even though the terminology we use is slightly different, our approach to capture a batch process expects the process model to be described as a pictorial flowsheet displaying the interconnections (as material flows) between unit procedures (or process steps). Each unit procedure (or procedure for short) is made up from a sequence of unit operations (or operations for short). The unit operation is the finest grain of modeling that can be represented by SuperPro Designer. Even though a unit operation's model may be a built-in sequence of process actions, the user may simply include or exclude some of these actions but we do not expect the user to configure their sequence. For example, a reaction operation may or may not include a gas sweep, a fermentation operation may or may not include aeration, etc., but the user simply chooses those actions as options on the operation's specification window without composing the sequence himself. Therefore, the unit operation is the finest grain of scheduling that is allowed by SuperPro Designer. The user can specify when an operation is assumed to start executing (start time) and how long it is assumed to last (duration). The start time of an operation can be set with respect to the start of the batch or with respect to the start (or end) of another operation anywhere in the same batch. The duration of an operation can be set explicitly or can be

calculated implicitly based on some rate parameter (e.g. the rate of transfer along with the material charged can dictate the charge time).

It is very important to understand that in SuperPro Designer, the simulation order of each unit operation is based on the flowsheet representation of the process (see 8.14f Partition & Sequencing) and not their relative scheduling sequence as set by the user. The recipe-level scheduling calculations (minimum recipe cycle time, number of batches per year, etc.) are always done after the mass & energy balances are finished. At that point, the actual start time of each operation is also calculated and their starting order is checked against the user's specifications for possible violations. It is possible that some of the M&E results may affect the outcome of the scheduling calculations since process durations may be calculated as part of the M&E balance calculations.

Typically a unit procedure maintains a sequence of several operations but there's nothing wrong with having a procedure only contain a single operation. In fact, the application represents continuous steps as a single-operation unit procedures (and will prevent you from adding any more operations to such continuous procedures). However, a unit procedure is not allowed to contain no operations.

Each unit procedure is assumed to be hosted by an equipment resource appropriate for that type of procedure (a chromatography procedure is hosted by a chromatography column, a vessel procedure by a vessel resource, etc.). Several procedures may be designated to use the same equipment resource (share equipment). Each unit procedure is represented by an icon and material interconnections between procedures are represented by streams between procedures. Operations and equipment do not have direct iconic representations on the flowsheet. Operations in a unit procedure can be accessed from the **Operation Data** submenu and equipment data can be accessed from the **Equipment Data** menu entry of the unit procedure's context (right-click) menu.

Material flows between procedures but it may also be retained by procedure states (or equipment contents). These states exist for unit procedures that are hosted by equipment resources with the ability to hold material (e.g. vessels). For such procedures, operations may also be viewed as transformations from one procedure state to another, often involving the influx of material from external streams and/or the removal of material onto procedure output streams. The modeling calculations for most of the operations do not involve the solution of differential equations but a set of algebraic equations that succinctly capture the overall performance of the operation without resorting to low level representation. Some models (by their nature) must involve such models (kinetic reactions, rigorous vapor-liquid calculations, etc.) However, the user can only introduce this complexity in a controlled manner and only in steps where such accuracy is of utmost importance.

BATCH VS. CONTINUOUS PROCEDURES

Some unit procedures, simply by the nature of the host equipment, cannot be run continuously. For example, a chromatography column. Typically, it is first equilibrated, then loaded for elution then washed/regenerated few times before the whole sequence is repeated. For such procedures, the continuous mode is not allowed (see Procedure Data Dialog: Scheduling Tab). For others, their operation is naturally perceived as continuous in time (e.g.a high-pressure homogenization or pumping) even though they can be started and stopped at any time (intermittent or semi-batch mode). Early on in the development of the simulation engine, it was recognized that unless we managed to smoothly integrate purely batch procedures (such as a

chromatography sequence) with a naturally continuous procedure (such as pumping) we would not be able to allow our users to capture a process in its entirety. SuperPro Designer's unique handling of flows between procedures, allows you to easily integrate a continuous step (such as distillation column) in a batch modelled process. You may also insert a batch unit (such as a batch reactor) in an otherwise continuously modelled flowsheet.

When a Batch Unit Procedure Functions in a Continuous Process...

Consider procedure P-10, a batch procedure, shown in the schematic interjected to operate in a continuous environment where all flows are specified and calculated on an amount-per-time basis (e.g. kg/h). Since the operation models contained in P-10 all expect an amount per cycle (batch) specification, the application's simulation engine presumes that each of the procedure's inputs and outputs is fed through a holding tank. Even though material flows in and out of the tanks continuously, the batch procedure P-10 functions in cycles. The holdup time (typically - but not always) in a setup like this must be given an appropriate value that cannot be less than the cycle time of the procedure but not exceedingly high as this will impose large sizing requirements. For more on the holdup time see 5.2a Holdup Time.

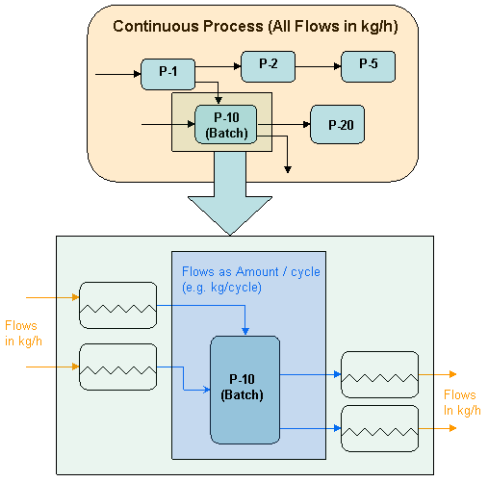


Figure 8.11: A Batch Procedure in a Continuous Process.

When a Continuous Unit Procedure Functions in a Batch Process...

In this case, all flows surrounding the continuous procedure P-10 (as shown in the schematic below) are set on a per-batch basis. Once again, we assume that the procedure is surrounded

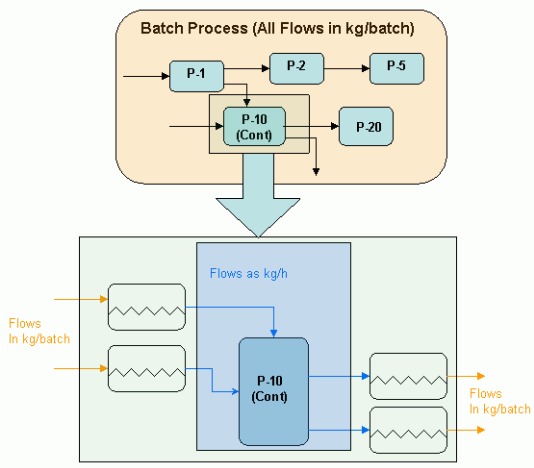


Figure 8.12: A Continuous Procedure in a Batch Process.

by holding tanks only this time, the holdup time doesn't need to be set by the user. The application presumes that the holding time is equal to the recipe's cycle time (time-between-batch-starts, see 7.1 Scheduling Terms & Definitions.)

8.14d Process Operating Mode: Batch vs. Continuous

The very first decision you will have to make when creating a new process simulation is to decide its **process operating mode**. The operating mode must be set to either batch or continuous. Even though SuperPro Designer can handle a mix of procedures (some operating in batch mode and some in continuous mode see 'Batch vs. Continuous Procedures' on page 8-31) it still needs to assume an operating mode for the entire process.

IF YOU CHOOSE BATCH AS THE PROCESS OPERATING MODE...

- All input specifications will be assumed that will be provided on a 'per-batch' basis. For example, material flows on input streams are (by default) expected to be supplied in units of 'kg/batch' or 'L/batch'. Some labor specifications are also expected to be supplied in hr/batch.
- Scheduling calculations will be performed at the conclusion of M&E balance calculations. All operations that execute in batch, will be showing a 'Scheduling' tab as part of their i/o simulation dialog. The user can set specifications on when they start (or finish) in relation to other operations in the process. The simulation engine will be followed by the scheduling engine. The scheduling engine attempts to calculate the cycle times and absolute start times for all the batch operations and procedures in the process. It will also calculate the minimum cycle time and the maximum number of batches (per year) for the

process (see 7.1 Scheduling Terms & Definitions). Finally it will perform a whole set of check-ups to verify that no scheduling constraint violations (such as equipment sharing) have been recorded.

- Every newly added procedure will be assumed to be performing in batch (or semi-continuous) mode. After the creation of the new procedure, this setting can be changed by visiting the Procedure Data Dialog.

IF YOU CHOOSE CONTINUOUS AS THE PROCESS OPERATING MODE...

- All input specifications will be assumed that will be provided on a 'per-h' basis. For example, material flows on input streams are (by default) expected to be supplied in units of 'kg/h' or 'L/h'.
- No scheduling calculations are performed. The 'Scheduling' tab will not appear as part of the i/o simulation dialog of operations (unless they participate in a unit procedure set to be executing in batch mode as an exception).
- Every new procedure capable of functioning in continuous mode will be assumed to be in continuous mode. Procedures hosted by equipment that operates inherently in batch mode (e.g. chromatography columns) will be assumed to be executing in batch / semi-continuous mode. For such procedures, the holdup time must be specified, see 5.2a Holdup Time.

You can always revisit the Process Operating Mode Dialog and change the plant's operating mode from batch to continuous (or vice versa) at any time. If you are switching from batch to continuous, then the program must switch all input specifications (such as input stream flows, consumption or labor rates, etc.) from 'per-batch' to 'per-h'. To make the conversion it will use the value of batch time at the time of conversion. It will also offer you the choice to switch the operating mode of all procedures currently included in the process and can perform in continuous mode. If you visit the Process Operating Mode Dialog to switch from continuous to batch, then all input specifications will be converted from 'per-h' to 'per-batch' assuming a 24hr batch time. You should visit all such input and adjust their values as they may not be accurate. The program will also give you a chance to switch the operating mode of all existing procedures from continuous to batch (or semi-continuous).

8.14e Countdown to Simulation Execution: The Pre-Simulation Checks

Before the application engages the simulation engine to carry out the M&E balance calculations, it needs to do a long list of checkup that need to all be passed before the simulation has any chance of succeeding. The list of checkup performed by the application is long and thorough. In fact, according to an un-official poll conducted by our tech support engineers, 9 out of 10 simulations never clear this point, so they are stopped before they even started. Here's the list of checks that are being done:

1. All batch procedures included in the recipe have at least one operation.
2. All operations included in procedures have been properly initialized by the user. In other words, the user has visited each operation's i/o simulation dialog and approved (exited with OK) their values.

3. All streams needed by the operations included in the process flowsheet are present. If there are any streams that are process inputs, they must be properly initialized.
4. There are no 'extra' streams in the process flowsheets. 'Extra' streams are streams that are not used by any of the operations currently present in the process.
5. There are no improper connections between procedures. Sometimes, the presence of operations that need special handling (back-propagation, see 8.14i Back-Propagation: Sources (Initiators) & Sinks (Terminals)) imposes some constraints onto the connectivity of procedures upstream from where the back-propagation starts. Also, when discrete entities are present (see 4.8 Discrete Streams), mixing up entities of different nature is not permitted.

Only when all of the above checks are cleared the application proceeds to the next step: the initiation of the simulation engine. If any of the above checks fails, a pertinent message is echoed in the error output window (see 8.17 Error Output Window).

8.14f Partition & Sequencing

After all pre-simulation tests are evaluated and passed (see 8.14e Countdown to Simulation Execution: The Pre-Simulation Checks), the simulation engine will engage. The simulation engine of SuperPro Designer follows the sequential modular approach. In other words, it considers first the procedure connectivity of the flowsheet (based on the material connections between procedures) and then it determines the order by which the engine will simulate (solve) the procedures, one by one. The order is decided in such a way that when solving a unit procedure all of its input streams are already known either because they are direct process inputs or because they are outputs of previously solved procedures. It should be emphasized that the solution order depends strictly on the material allocation scheme as demonstrated by the stream connectivity. It is important to note that even for processes set to operate in batch mode, timing (or scheduling) considerations are not taken into account when solving the M&E balances. If there are more than one independent chains of unit procedures (like the scheme shown below), it is not known a-priori which one will be ordered first (in the solution sequence).

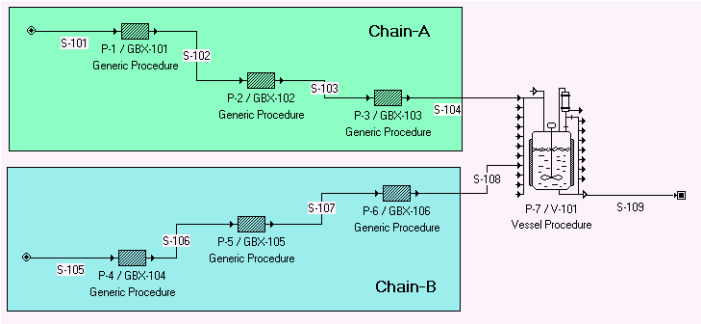


Figure 8.13: Simple Procedure Sequencing.

In other words, for a situation like the description above, the solution sequence could be:

(a) P-1, P-2, P-3, P-4, P-5, P-6, P-7 or

(b) P-4, P-5, P-6, P-1, P-2, P-3, P-7

Note that in either case, the final outcome of the simulation will be the same.

When each procedure is solved, all operations inside that procedure are solved in order that they are specified by The Operation Sequence Dialog. After the end of the simulation, the actual start times of each operation are calculated (based on their scheduling specifications and the start and end times of other operations that they may use as reference). If the start times of two operations that appear in a unit procedure's sequence do not agree with their relative order, an error will be generated.

When loops are present the above simple-sequence solution scheme will not work since it is impossible to find such a sequence where all inputs are known by the time each procedure is

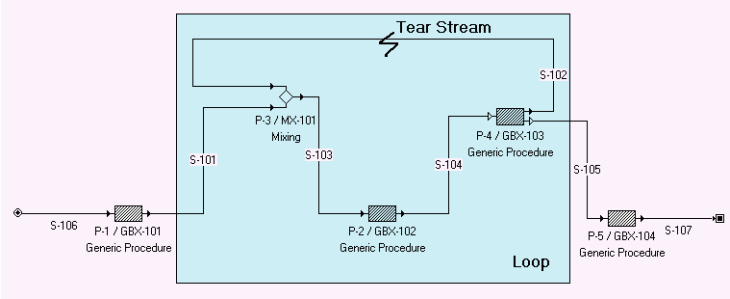


Figure 8.14: Loop Identification and Tear Stream Selection.

about to be solved. For instance, in the (simple) example shown above, one can argue that P-1 is to be solved first, but then, there are no other steps with known inputs so that they can be queued next in the solution order. Instead, the group of { P-2, P-3 and P-4} must be solved next, and finally P-5. In such cases, the simulation engine will generate a partition or a composite block of unit procedures that are all interdependent (i.e. they reside on the same loop(s)). The simulation engine will still have to make sure that the solution of this new partition will be properly sequenced with respect to the rest of the flowsheet's pieces (whether they may be simple procedures or other partitions.

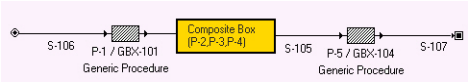


Figure 8.15: Composite Boxes (Solved Iteratively) Sequenced with Simple Procedures.

Once all partitions are identified and properly sequenced, the simulation will proceed to solve in the specified order. Of course, solving a partition requires some sort of iterative scheme, as described in 8.14g Loop Identification and Tear Stream Selection.

8.14g Loop Identification and Tear Stream Selection

After the partitions have been identified, the simulation engine must decide on an iterative solution strategy on how to solve them. Consider a sample flowsheet shown below:.

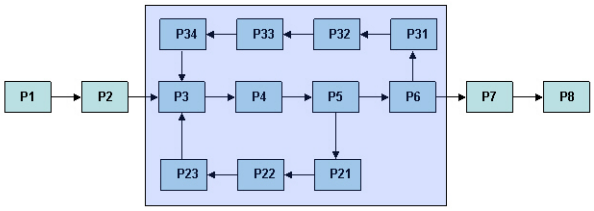


Figure 8.16: Partition Identification.

Clearly the group of P3,P4,P5,P5,P21,P22,P23,P31,P32,P33,P34 must form a partition (let's call it CP) and solved iteratively. The overall sequence will be P1,P2, CP, P7,P8.

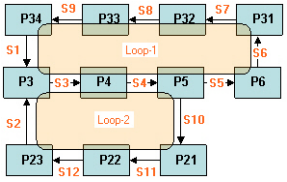


Figure 8.17: Loop Identification in a Partition.

In order to prepare for the solution of CP, the simulation engine must analyze the connectivity inside the partition and then identify all independent loops. Then, it must chose the 'best' tear stream set that cuts all the loops in a way that lends itself in the most favorable computational effort. It turns out that in most cases, the tear stream set that has such properties is the so-called 'Non-Redundant Tear Stream Set' that satisfies the following two constraints:

1. No loop is cut more than once.
2. The number of tear streams is as small as possible.

Here's how the simulation engine searches for such sets: Each loop is identified by its sequence of links. For example, the partition shown above features two loops:

L1: S3,S4,S5,S6,S7,S8,S9,S1 and

L2: S3, S4, S10, S11, S12, S2

The above information is kept as a stream incidence matrix for each loop. Reversely, each segment, can be assigned an index that designates in how many loops it appears. This index is called the Loop Occurrence Index (LOI for short). For example, S1 appears in only one loop, so its LOI is 1. However, S3 and S4 appear on both loops, so their LOIs are 2. Based on such information generated for all the streams (links) and their participation in the formation of loops, the simulation engine uses the following strategy:

1. Identify the loop incidence matrix for all remaining loops.
2. Order all streams based on their loop occurrence index (LOI).
3. Chose the head of the list as the next tear stream; if there's a tie, chose randomly but if the strategy fails to find a set, come back to this point and chose the next available candidate.

4. Remove all loops that are torn by the chosen candidate stream and then remove from the loop incidence matrix all streams that participate in these loops and nowhere else.
5. Repeat until either no more loops are left untorn (success) or no more candidates are left to chose (but at least one loop still remains untorn). In the latter case, the search algorithm attempts to backtrack and chose the next best candidate and continue.

In order to exhaustively search for all possible candidate streams till a Non-Redundant Tear Stream Set is found, it may take a very long time (depending on the size and complexity of the loops in the specific flowsheet). In fact, it is possible that even if all possible candidates are searched such a set is never found (doesn't exist). Of course, if the above algorithm fails to find a non-redundant set of tear streams, it reverts to the simpler search for finding any set of tear streams (that is very fast and always possible). If your particular connectivity features a very involved loop structure, below are a few tips on how to tweak the loop identification strategy of SuperPro Designer that may lead to faster simulation completion:

Tip#1: During Step#2 of the search algorithm above, instead of picking the next-best available candidate, instruct the search engine to only pick the best candidate(s): that is the stream(s) with the highest loop occurrence index (LOI).If after choosing those streams as candidates the search fails, allow the engine to fall back to non-redundant sets.

Tip#2: To improve overall search performance, instruct the algorithm to record all failed choices so that it doesn't repeat the same mistakes twice in its search for the non-redundant set. This choice may improve performance in finding a non-redundant set of tear streams.

Tip#3: Allow the engine to directly search for and accept any tear stream set (even if it turns out to be a redundant set). A redundant set of tear streams may require longer times to converge the iterations, but overall, since the identification of non-redundant tear stream sets may be very expensive, the entire solution may conclude in much less time.

All of the above tweaks to the loop identification algorithm can be made from the Recycle Loop & Tear Stream Options Dialog that appears when you select **Recycle Loop & Tear Stream Options** from the flowsheet's context menu.

Returning to the example chosen earlier, a non-redundant set of tear streams is either {S3} or {S4}. Notice that either one of those single streams cut both loops (L1 & L2), see Figure 8.18.

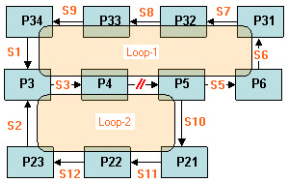


Figure 8.18: Non-Redundant Set of Tear Streams : {S4}.

A tear stream set such as {S1, S2} is not non-redundant since it does not feature the minimum number of tear streams (2 instead of 1), see Figure 8.19. Also, a tear stream such as {S4, S5} is also not a non-redundant set because (a) it has more than the minimum number of tears, and (b)

it cuts L1 twice. However, sometimes a set like {S1, S2} may be preferable as streams S1 and S2 may be better candidates for guessing their contents, or because their choice as tears implies

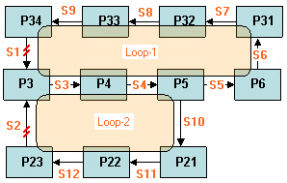


Figure 8.19: Redundant Set of Tear Streams: {S1, S2}.

a solution sequence that may be preferable. For such cases, the application allows you to 'bias' or even force your preferences for tear stream candidates. You can select **Preferred Tear** from a stream's command menu to direct the tear identification algorithm to chose that stream as a tear. Of course, you can only assign as many tear streams as the number of independent loops that exist.

References

1. A. W. Westerberg, H.P. Hutchison, R.L. Motard & P. Winter (1990) Process Flowsheeting, Cambridge University Press.

8.14h Convergence Strategy

After a set of tear streams has been identified, the simulation engine prepares for the iterative calculations as follows:

1. Zeroes all intermediate streams except those selected as tear streams.
2. Generates an initial 'guess' for the state variables x_1, x_2, x_3... x_n(composition flows and temperature) for each tear stream. The tear stream initialization policy can be chosen by the user as one of the following:
   (a) Keep their current values (as resulted from last simulation)
   (b) Reset all compositions (and component flows) to zero and temperature, pressure to ambient, or
   (c) Allow the user to provide his/her own guess for each tear stream.
3. Solves all the elements in each partition in the predetermined order until a new set of values is generated for all the tear stream variables: $g(x_1)$, $g(x_2)$, $g(x_3)$... $g(x_n)$.
4. Based on the originally guessed values (x_1, x_2, x_3... x_n) and the generated values ($g(x_1)$, $g(x_2)$, $g(x_3)$... $g(x_n)$) produce a new set of values to try.
5. Check to verify if the generated set of stream state properties are 'sufficiently close' to the guessed set of states. In that case, we declare that convergence has been achieved and we end the iteration. If that is not the case, then we generate another set of guesses and repeat steps 4 and 5 until (a) convergence has been achieved or (b) the maximum number of iterations is exceeded.

If the last attempt to solve the M&E balances failed (solution did not converge) because the convergence was making progress but not enough before the number of allowable iterations was exhausted, then the above strategy will actually be very beneficial for the next attempt to solve the M&E balances. If, on the other hand, the solution of equations was diverging, the above strategy will only exacerbate the problem. In that case, users are advised to instruct the simulation engine to reset the tear stream initial guesses to zero and start over. From version 8.0 the user also has the option of providing his/her own set of values to be used as initial guesses for the tear streams.

GENERATING THE NEXT GUESS

The most commonly used method for generating the next guessed value x_n (when one or more previously guessed values x_{n-1}, x_{n-2},... are known) is simple successive substitution. In other words, if for a given value x_{n-1} the calculated value is $g(x_{n-1})$ this value is used as the next guess x_n: $x_n = g(x_{n-1})$.

Sometimes the successive substitution method may lead to a diversion. Consider solving the function g(x) shown below (Figure 8.20):

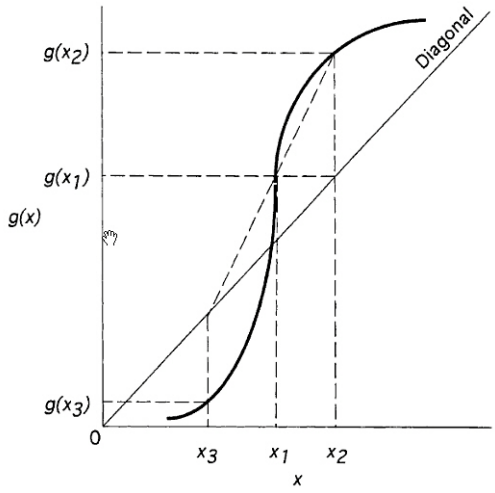


Figure 8.20: Wegstein's Next Guess Estimation.

Following the successive substitution method, after guessing x_1 first it produces $g(x_1)$ as the next guess and then using that as x_2 the calculated value of $g(x_2)$ clearly the algorithm appears to diverge from the solution (x = g(x)). On the other hand if one uses as the next guess the intersection between the line defined by the two points (x1, g(x1)) and (x2, g(x2)):

$$\frac{y - g(x_1)}{x - x_1} = \frac{g(x_1) - g(x_2)}{x_1 - x_2} \qquad \text{eq. (8.6)}$$

and the line defined by y = x, it will arrive as the next guess point x3 as:

$$x_3 = \frac{x_1\, g(x_2) - x_2\, g(x_1)}{x_1 - x_2 - g(x_1) + g(x_2)} \qquad \text{eq. (8.7)}$$

or, if we define as q the slope of the Wegstein line:

$$q = s/(s-1)$$
$$s = \left[g(x_1) - g(x_2)\right]/(x_1 - x_2) \qquad \text{eq. (8.8)}$$

then:

$$x_3 = q\, x_2 + (1-q)\, g(x_2) \qquad \text{eq. (8.9)}$$

Typically, q is bound by an upper value (q_{max}, defaults to +5) and a lower value (q_{min}, defaults to -5) to avoid leading itself to instability. If the convergence procedure seems to be unstable, raising the value of q_{min} (i.e., making it less negative) may improve convergence; if it is converging very slowly but monotonically, you might lower q_{min}; and if it is converging in an oscillatory manner, try raising q_{max}. You also have the option of setting the value of q to a fixed value. If q is set to 1 then the algorithm matches exactly a successive substitution; if q is set between 0 and 1, then the procedure is a modified successive substitution; if q is negative then the convergence is accelerated. The technique to be used when generating the next guesses during iteration is set from the Recycle Loop & Tear Stream Options Dialog.

CONVERGENCE CRITERION

The interpretation of when a guessed state for a stream is ‘sufficiently close’ to the generated (calculated) state of the same stream amounts to what is called the convergence criterion and it can be adjusted as follows:

The ‘closeness’ between a guessed value for a variable and a calculated value is measured as the relative deviation between the two values:

Relative Deviation (RD) = Abs. Value { (Guessed Value - Calculated Value) / Guessed Value }

When the relative deviation for an independent variable is lower than a set tolerance, the variable is considered as converged.

1. Setting the tolerance value to lower values, will enforce a tighter matching between the guessed and calculated values (and therefore will allow for smaller errors) but it may take longer to converge.
2. The user may decide to consider only the total mass of streams as the independent variables where the convergence criterion is applied. Alternatively, each individual component flow is considered and unless they all satisfy the convergence criterion, the iterations continue.
3. A stream’s state may or may not include its temperature. If you exclude temperature variations then inaccuracies due to non-closing energy balances are not considered as

reasons to continue the iterations. This relaxed criterion may be a good starting point for simulations that may fail to converge initially when all mass flows and temperature are considered as independent variables.

The user may monitor the progress during successive calculations in the iterations for recycle loop convergence. The simulation engine records in a file the values of all the variables that are being monitored and allows the user to inspect them after the calculations ended (either due to exceeding a maximum number of iterations or due to managing to bring all variables under tolerance limits). This feature can be turned on by checking the "**Record Convegence Progress**" box in the Recycle Loop & Tear Stream Options Dialog.

The setting for the relative tolerance to be enforced between consecutive guesses, as well as which parameters to consider during iterations can be adjusted from the Recycle Loop & Tear Stream Options Dialog that appears when selecting **Recycle Loop & Tear Stream Options** from the flowsheet's command menu.

8.14i Back-Propagation: Sources (Initiators) & Sinks (Terminals)

Oftentimes during modeling, the need arises to have an operation dictate the amount of material that it needs to receive on a stream in order to perform its task. For instance, consider the Nutsche filtration procedure below.

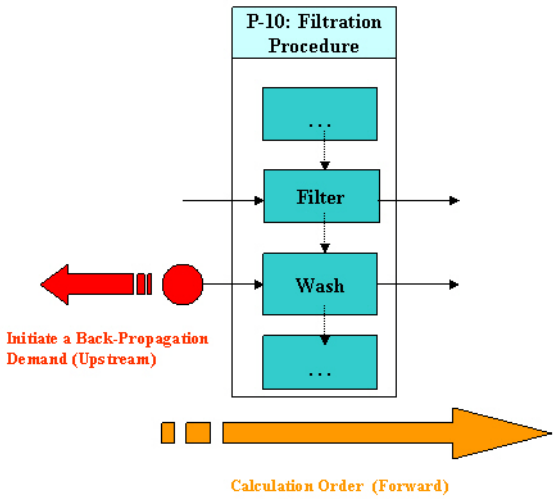


Figure 8.21: Back-Propagation Demand Travels Opposite the Normal (Forward) Calculation Order.

Typically after the filtration operation itself, there's a need to wash the accumulated cake and the demand for solvent is usually set as a multiple of the amount accumulated in the cake. Since that amount is not known until the simulation sequence reaches this procedure and passes the filter operation, then the amount of the material required to be present on the wash (input) stream is not known either. In such a case, when the simulation engine reaches the wash operation, it will use whatever composition and amount exists on the wash stream but it will attempt to scale up the amount in order to meet the demands as expressed by the user's request (in this case to meet the wash amount/cake amount ratio). This will create a discrepancy between the amount as computed (and set) on the wash stream by the forward calculation (material demand) and the current state of inputs / operations upstream (if any, as calculated by

the solution of procedures earlier in the calculation order) leading to the wash stream's flowrate. In the SuperPro Designer's simulation engine, a **back-propagation source** (or BPG source for short) has been reached. If the wash stream happens to be a direct process input stream with its 'auto-adjust flow' flag checked, then the simulation engine will scale the total flow of that stream to meet the material demand. Then, the simulation will proceed to the next procedure after the filtration. If the wash stream is not a direct input to the process but an intermediate (i.e. it originates from another procedure) then the simulation engine must initiate a **back-propagation material demand** through the upstream network of streams and/or procedures until it reaches a location where the demand can be met (a **back-propagation terminal**, or BPG terminal for short). Such BPG terminals are:

1. A pull-out operation's output stream.
2. An input stream with the 'auto-adjust flow' flag turned on.

As the back-propagation demand travels upstream, as soon as one of the two possible BPG terminals is reached, the simulation engine considers the back-propagation demand as successful, as it manages to reconcile the material demand requested by the BPG source (wash operation in our case).

In order for this back-propagation mechanism to work, the simulation engine needs to successfully pass the generated demand (red ball above) through all upstream vessel states

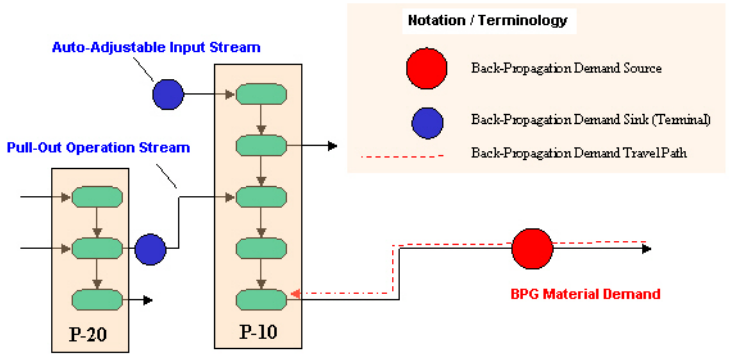


Figure 8.22: Back-Propagation (BPG) Sources (Initiators) and Sinks (Terminals).

and material streams (shown in green in the schematic above) until it reaches points that can absorb (i.e. satisfy) the demand (blue points above). In order for this mechanism to work, certain connectivity rules must be obeyed.

The most important premise that these rules are trying to protect is the following:

- Material demand must only be propagated backwards without generating any forward disturbance(s).

For example, consider the path the BPG of material demand is following in the schematic below (Figure 8.23). The path goes through procedure 'P-20' and then through 'P-10' all the

way to its (single) input stream without the possibility of traveling forward (the single output stream from 'P-10' is a process output and not an intermediate - that would not be allowed)

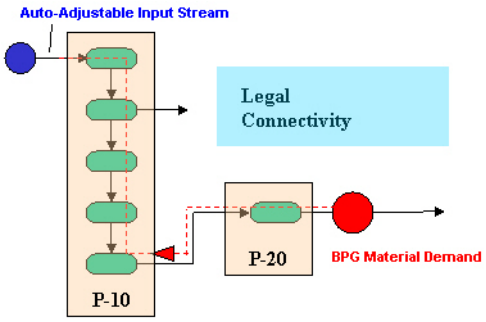


Figure 8.23: Legal Back-Propagation Connectivity.

This rule, of course, only comes into play if the demand must be propagated through procedures/operations. If that is that case, no operation along its path should affect a procedure output stream that carries material to another procedure down stream (seeFigure 8.24 below).

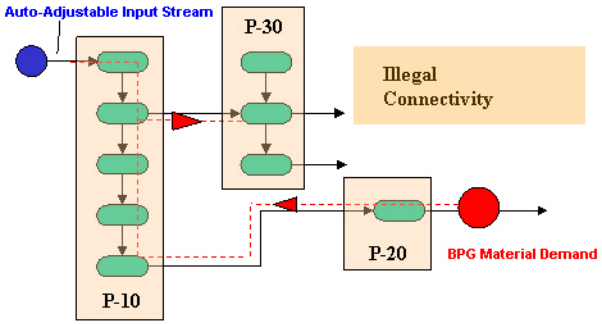


Figure 8.24: Illegal Back-Propagation Connectivity (Allows Forward Travelling of BPG Demand).

Any connectivity that will allow the material demand to propagate forwards is not allowed (will be detected by SuperPro Designer's connectivity check before simulation is carried out and will result in an 'Illegal Connectivity' error message echoed in the Error Output Window.

IF THE MATERIAL DEMAND ORIGINATES ON A PROCESS INPUT...

If the stream whose flow is the original source of the generated material demand (like, the wash stream of the Nutsche procedure in the above example) is a direct process input, then the user must:

(a) Set the composition of that stream

(b) Leave the total flow of the stream as set by application. Notice how the total flow can no longer be set by the user. Also notice that the 'Auto-Adjust Flow' flag on the stream is automatically set by the application.

IF THE MATERIAL DEMAND ORIGINATES ON AN INTERMEDIATE STREAM...

If the stream originating the back-propagation material demand is a process intermediate and assuming that the back-propagation demand network reaches input streams, then the user must:

(a) Set the 'Auto-Adjust Flow' flag for all such input streams, and

(b) Set the composition for all such input streams, and

(c) Set least one of them to a non-zero flow. It is recommended that all flows are set to non-zero flow amounts. If the relative amounts of flows are of importance (since they may dictate the composition of intermediate streams) then all such auto-adjustable input streams must be set.

For an example that demonstrates the above principles, see 'Back-Propagation of Material Demand: An Example' on page 8-45.

BACK-PROPAGATION OF MATERIAL DEMAND: AN EXAMPLE

Sometimes the simulation sequence may proceed in a seemingly opposite direction than one may expect. For instance, consider the case displayed below:.

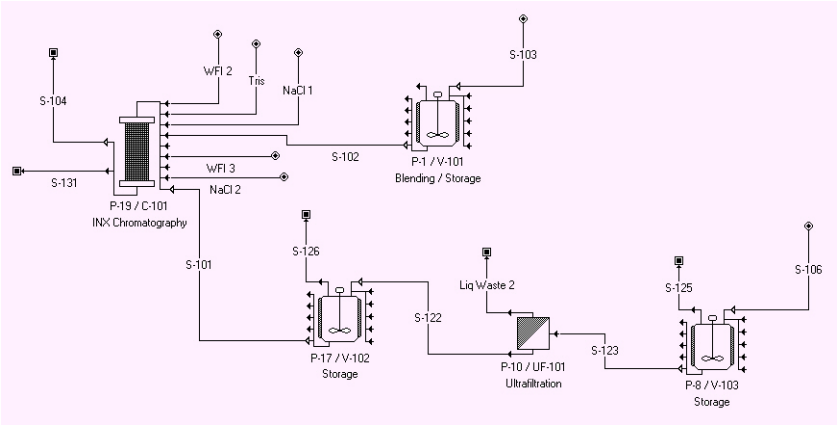


Figure 8.25: An Example Process with Back-Propagation.

One may expect that the sequence would be: P-8, P-10, P-17, P-1, P-19. However, what will actually happen is the following: P-8, P-10, P-17, P-1, P-19, P-1, P-19. Notice that after solving the forward sequence as expected, the simulation stepped backwards to P-1 and then forward again to P-19. The reason that this backward-then-forward sequence happened is the following: As part of the solution of P-19, one (or more) wash operations in that unit procedure adjust the flow of incoming stream S-102. As the wash amount depends on operating parameters set in the wash operation's i/o simulation dialog, the actual amount of flow on stream S-102 is adjusted properly only after the simulation engine has passed through P-19 (Chromatography Step). However, once the flow on S-102 has been adjusted, the simulation engine must 'back-propagate' the effects of this change to all unit procedures (and their operations) upstream from stream S-102. Thus, P-1 (in our case) is revisited and resolved. If there were more unit procedures upstream from P-1, they would have to be re-solved as well.

The main objective of this back-propagation mechanism employed by SuperPro Designer is to pass the extra material requirements imposed by an operation somewhere in the flowsheet, upstream at a place where the demand can be satisfied. As explained in more detailed elsewhere (see 8.14i Back-Propagation: Sources (Initiators) & Sinks (Terminals)) there are two possible ways that the extra demand can be satisfied:

(a) The upstream path leads to a stream associated with (or manipulated by) a Pull-Out operation (see Pull Out: Modeling Calculations.) In that case, the operation's simulation has the ability to adjust the amount of material pulled out of the contents of a vessel in order to satisfy the requirement (provided there is enough amount in the vessel). Since the amount in the vessel after the pull-out operation has adjusted its output, will be modified, all operations in the UP's queue past the pull-out operation must be re-solved. The back-propagation mechanism will fail, if there are operations down the UP's queue that may propagate the effects of the adjusted vessel contents forward (e.g. a transfer out where the amount is set to be a percentage of vessel contents). In that case, SuperPro Designer will generate an error.

(b) The upstream path leads to one (or more) input streams that all have the 'Auto-Adjust' flag for their flowrates on.

If neither (a) nor (b) are present on a back-propagation path, the application will bring up an error message.

SuperPro Designer's solution manager will generate an error message if the upstream connectivity from a stream whose flow is the source of a back-propagation demand, is not appropriate. There can be many reasons why the upstream connectivity of such a stream may not be appropriate (i.e. do not allow back-propagation). The most common reason is that the user neglects to set the 'Auto-Adjust' of an input stream. For instance, in our example above, if the user neglects to set the flow of S-103 to 'Auto-Adjust', then an illegal BPG connectivity message will be echoed.

8.15 SIMULATION BREAKPOINTS

When simulating a large process, oftentimes the outcome is not what a user may expect. The calculations may end up in an abrupt stoppage, or they may conclude but the outcome may not be what a user may expect. Typically the calculations will go wrong first in some unit procedure (or more specifically in one of a unit procedure's operation outcomes) and then, they will be propagated downstream to others perhaps leading to a chain of warnings and/or error messages. The use of breakpoints can greatly facilitate the detective work that needs to be done in order to locate where things start to go wrong.

Placing a breakpoint somewhere in the process, is similar to placing a red-light in the streaming of the simulation calculations. As soon as the simulation engine of the application sees the red light, the simulation engine comes to a screeching halt, and awaits further instructions from the user as to what to do next. Since the simulation engine executes the solution of the entire process by solving one procedure at a time, it makes sense to allow users to place breakpoints around a unit procedure. You can place a breakpoint within or around a unit procedure by visiting the its Breakpoints Dialog (select **Set Breakpoints** from the procedure's context menu). You request the simulation engine to stop:

1. Right before the calculations in this procedure are about to begin (upon entering) and before any auto-initialization may be executed (see below).
2. Right after automatic material pull-in or auto-initialization (if applicable, see 5.5a Default Input Ports & Auto-Initialization)

3. Before any of the operations that appear in the unit procedure's queue.
4. Before the automatic material push out or auto-removal (if applicable, see 5.5b Default Output Port & Auto-Removal)
5. Right after the calculations in this procedure are finished (upon exit).

To indicate that a breakpoint has been placed in or around a unit procedure, the application will display an indicator ( ) above the procedure's icon.

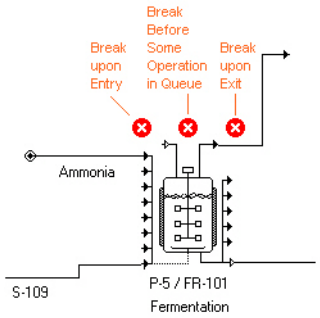


Figure 8.26: Breakpoints Indicators Around a Unit Procedure Icon.

If the breakpoint is placed upon entering the procedure's calculations, then the breakpoint indicator is shown near the entry side of the procedure; if the break in the calculations is to happen after the ending the calculations in one of the contained operations, then the breakpoint indicator shown above the procedure and in the middle. Finally, if the breakpoint is placed to force the calculations to stop right after the end of the procedure's simulation, then the breakpoint indicator shows above the procedure's icon and near the exit side of the procedure. Sometimes you may need to temporarily de-activate a breakpoint but without removing it (see Breakpoints Dialog). If a breakpoint has been deactivated it shows grayed out ( ).

When the simulation engine reaches a breakpoint and stops, SuperPro Designer displays a status icon under every unit procedure in the process. For the unit procedure that forced the calculations to stop, the indicator is one of the following:

the simulation calculations have stopped right after entering this procedure

the procedure calculations have stopped before one of the operations in the queue

the simulation calculations are stopped right before exiting this procedure

For all other procedures (other than the one where the active breakpoint exists), here are the possible indicators and their meaning:

the procedure has not been visited yet

the procedure has been successfully simulated already

the procedure is being solved recursively (as part of loop convergence)

the procedure solution ended unsuccessfully (as part of an un-converged loop)

the procedure solution ended unsuccessfully (an error was encountered)

When the simulation engine is stopped in the midst of its calculation sequence, you can view the values of streams on the stream summary toolbar (see 8.11 The Stream Summary Table) or visit any of the process elements i/o simulation dialogs (unit procedures, operations, streams, equipment, equipment contents, etc.) and inspect (even change) their property values. If you do change values, then note that the new values will only affect the outcome of the simulation if they are applied to operations in procedures that have not been solved yet (in other words, the indicator shows underneath). Changing values on procedures that have already been solved will only affect the outcome of the next simulation run.

When dealing with breakpoints, the simulation toolbar and all the options that presents, are very important. Each button on the toolbar can direct the simulation engine what to do next: it can move on to the end of the next operation, or at the end of the current procedure, or directly to the beginning of the next procedure; you can even stop the simulation altogether or skip right through to the next breakpoint. You can show/hide the simulation toolbar by selecting **Simulation Control ▸ Toolbar** from the **View** menu. For more details, see 8.16 Simulation Control Toolbar.

*After going through several debugging sessions where the simulation engine reaches (one or more) breakpoints and is controlled manually by the user, one may find it necessary to make a run where the engine doesn't stop at the preset breakpoinst, but attempts to complete the calculations from beginning to end without a stop. For this reason, there's an entry in the flowsheet's context menu (**Breakpoints ▸ Deactivate All**) that will de-activate (without removing) all the preset simulation breakpoints. Later you may visit the same menu and this time chose **Breakpoints ▸ Activate All** to re-activate all existing simulation breakpoints. Note that once one or more breakpoints have been set, you can quickly remove them all by selecting **Breakpoints ▸ Clear All** from the flowsheet's context menu.*

8.16 SIMULATION CONTROL TOOLBAR

The simulation control toolbar (Figure 8.27) is shown by clicking on the **Show/Hide Breakpoints** button ( ) on the main toolbar or by selecting **View ▸ Simulation Control ▸ Toolbar** from the main menu. The buttons on the toolbar may or may not be active

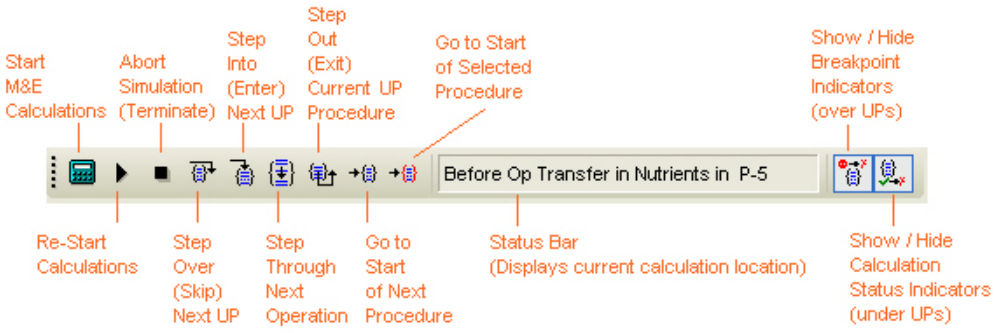

Start M&E Calculations
Abort Simulation (Terminate)
Step Into (Enter) Next UP
Step Out (Exit) Current UP Procedure
Go to Start of Selected Procedure
Show / Hide Breakpoint Indicators (over UPs)
Before Op Transfer in Nutrients in P-5
Re-Start Calculations
Step Over (Skip) Next UP
Step Through Next Operation
Go to Start of Next Procedure
Status Bar (Displays current calculation location)
Show / Hide Calculation Status Indicators (under UPs)

Figure 8.27: The simulation control toolbar.

depending on the state of the simulation engine. The simulation engine can be in three possible states:

1. **Idle**: The status bar will indicate the message: "Waiting for simulation to start...'
2. **Running (Auto)**: When no breakpoints are set (or they are all deactivated), the simulation engine will run on 'automatic control'. In other words, the order of calculations is set (see 8.14f Partition & Sequencing) and the calculations proceed from beginning to end without any user intervention.
3. **Running (Manual)**: When a breakpoint is met, the engine gets into 'manual control mode'. It pauses and awaits the user's next command as to what to do. In that case, the buttons available on the simulation control bar come into place as they can be used to instruct the engine what to do next (see below).

Active when the simulation calculations have not been started yet. Clicking on the button will initiate the mass & energy (M&E) balance calculations; it is equivalent to clicking on the same button on the main toolbar or selecting **Tasks ▸ Solve M&E Balances** from the main menu.

Active when the simulation has been paused due to reaching a breakpoint. If you click on this button, the simulation engine will restart and it will pause again when either another breakpoint is encountered or the end of the simulation calculations has been reached

Active when the simulation calculations have on-going or they have been paused due to reaching a simulation breakpoint. Clicking on this button will stop the simulation engine and abort the calculations without going through the procedures still unvisited in the simulation order

Active when the simulation engine has stopped due to reaching a breakpoint, and the stop location is right before (upon entry) of a unit procedure. Clicking on the button will force the engine to go through all the calculations in the procedure (without stopping anywhere) and then pause upon exiting the procedure

Active when the simulation engine has stopped due to reaching a breakpoint and the stop location is right before (upon entry) of a unit procedure. Clicking on the button will force the engine to step into the procedure's calculations, and execute the auto-init (if active) or execute the first operation's solution.

Active when the simulation has been paused and the stop location is somewhere inside a unit procedure (i.e., right before an operation) and there is at least one more operation in the procedure's queue that has not been solved yet. Clicking on the button, will force the engine to go through the calculations of the next operation in the current procedure's queue and pause again.

Active when the simulation engine has stopped due to reaching a breakpoint, and the stop location is right before (upon entry) of a unit procedure. Clicking on the button will force the engine to go through all the calculations in the procedure (without stopping anywhere) and then pause upon exiting the procedure.

Active when the simulation has been paused and the stop location is somewhere inside a unit procedure (i.e., right before an operation). Clicking on the button, will dictate the simulation engine to continue through all the calculations in this procedure, solving all operations in the queue, and then it will pause upon exiting the procedure.

Active when the simulation has been paused and the stop location is anywhere (before, during or after a unit procedure). It will restart the engine and force it to stop right before entering the next procedure in the order of calculations.

Active when the simulation has paused (due to a breakpoint) and there's a single selected procedure that has not been visited yet by the simulation engine. If clicked, it will restart the engine and force it to stop right before entering the calculations of the selected procedure (provided no other breakpoints forced the engine to stop prior to that). It amounts to setting a 'once-only breakpoint' upon entry of the selected procedure.

When pressed, the application displays under each procedure the status of calculations in the procedure at the time that the simulation engine is paused (after reaching a breakpoint).

If pressed, then the application will display the breakpoint indicators (for active breakpoints and for inactive breakpoints) over the procedures where they are set.

8.17 ERROR OUTPUT WINDOW

Every user's dream is to complete a simulation within a few minutes by adding their components of choice, inserting the procedures and operations necessary to represent their process, connect them with streams, initialize the operations and the input streams, click on the **Solve M&E** button ( ) and be done! Unfortunately in real life this never happens. Users often make mistakes on several levels: they forget to include necessary streams; they neglect to initialize all the operations; they provide initialization conditions that lead to infeasible results, etc. Fortunately, the application performs hundreds of checks to make sure that structurally all the pieces are in place before we execute the mass & energy (M&E) balances (or any other action for that matter). Then a whole other set of numerical checks may need to be passed. After the calculations finish, another set of checks may be performed to make sure the results are in valid ranges. Inevitably, something will go wrong often. For all the issues that may be encountered, the application uses an output pane (the 'error output window', see Figure 8.28)

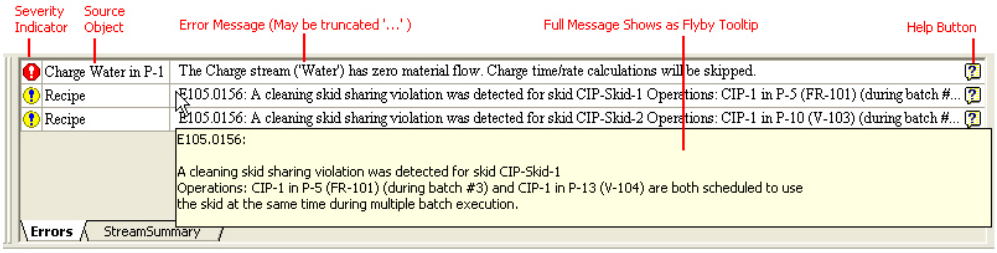

Severity Indicator
Source Object
Error Message (May be truncated '...')
Full Message Shows as Flyby Tooltip
Help Button
Charge Water in P-1
The Charge stream ('Water') has zero material flow. Charge time/rate calculations will be skipped.
Recipe
E105.0156: A cleaning skid sharing violation was detected for skid CIP-Skid-1 Operations: CIP-1 in P-5 (FR-101) (during batch #...
Recipe
E105.0156: A cleaning skid sharing violation was detected for skid CIP-Skid-2 Operations: CIP-1 in P-10 (V-103) (during batch #...
E105.0156:
A cleaning skid sharing violation was detected for skid CIP-Skid-1
Operations: CIP-1 in P-5 (FR-101) (during batch #3) and CIP-1 in P-13 (V-104) are both scheduled to use
the skid at the same time during multiple batch execution.
Errors
StreamSummary

Figure 8.28: The error output window.

to echo its complaints. The error output window is initially hidden, since there's nothing to be displayed. As soon as the application wants to echo a message the error window shows as a separate tab ('Errors') on the same toolbar that the stream summary table appears. Since there may be more than one messages that are detected, the window may present multiple lines (each

line corresponds to a message). Notice that the messages appear to show on a grid that has four columns:

1st Column	Severity Level Indicator Warning: an unexpected value or situation was encountered; the original command concluded but the validity of the results may be questionable. It is up to the user's discretion as to whether the warning warrants further investigation or it can be safely ignored. Non-Severe Error: An error was encountered but the application managed to bypass it and continue on with the original command. The circumstances reported by the application need to be addressed otherwise the results may be (at least partly) incorrect or incomplete. Severe Error: An abnormal situation was encountered that prevented the application from concluding the original command issued (e.g. show a graph, or do the M&E balance calculations, etc.) The user's attention is needed before any progress can be made on this issue.
2nd Column	A short descriptor will be shown that indicates the source of the warning/error. For example, the displayed text could be the name of a stream, unit procedure, operation, equipment resource, etc. or it could simply be 'process' or 'RepEng' (for reporting engine), or 'SimEng' (for simulation engine) etc. The tooltip displayed when the mouse is over the column may display a more detailed description of the error/warning source.
3rd Column	The error/warning message's text is displayed as a single line string in this column. Typically, the string will have two parts: the first part is a message ID in the form of: E***** (for errors) or W***** (for warnings). This ID makes it easy to convey the message to our technical support engineers should the situation persists and the user is unable to circumvent the issue without help. The rest of the message, is a verbal (short) description of the situation encountered. As space may not allow, the entire text may not be visible in the 2nd column. If that's the case, the message is shortened and ellipsis will be shown at the end of the displayed text. If you move your mouse over the text, the message in its entirety will be displayed as a tooltip.
4th Column	If you see this button at the end of the message, it implies that a specific topic for this message exists in the help system of the application. Clicking on this button, will fire up the help engine (if it's not already running) and present information about this topic. Sometimes more explanation is presented in this context as well as tips on how to resolve the issue (along with links to related topics in the help system).

The error output window can be shown or hidden by clicking on the **Toggle the Error Output Window** button ( ). When the tab is showing you can also right-click over the window and select **Hide** from its command menu.

The error output contents are automatically cleared before a new command (that may generate messages) is issued. If you wish to clear its contents manually, you can select **Clear Errors/Warnings** from the window's command menu. You may also print the contents of the window by selecting the **Print** command from the context menu.

FILTERING WARNING & ERROR MESSAGES

By default, the application will allow all messages at the level of (user) 'Warning' or below to be echoed and therefore visible to the user. It is possible that during the execution of lengthy and complex solution algorithms, some issues may have been encountered that were not severe enough to trigger a user-level warning or error message. Essentially, the application's logic was able to recover and adjust accordingly. However, such messages (termed 'Internal Warning' or 'Internal Error' messages) may at times be a good indicator of possible unexpected behavior of the calculation engine. Since those messages are not typically of interest to the user, they are not shown unless you lower the error/warning threshold of the error output window. This is done by selecting **Set Error/Warning Threshold** from the window's command menu, see 8.22z Error / Warning Output Filter Threshold Dialog.

8.18 OTHER (MISC.) PROCESS PROPERTIES

Currently, the following options exist under the category of 'Miscellaneous' (they can all be accessed and changed from the Miscellaneous Process Preferences Dialog (select **Preferences ▸ Miscellaneous** from the flowsheet's context menu).

8.18a Show Page Breaks

Turn on this option to display directly on the flowsheet the boundaries of pages.

If this option is checked, then the application will display on the flowsheet the boundaries of pages as a red dotted line. This marking may help the designer rearrange the location of icons and / or streams so that when printed on the selected paper size and orientation the drawing is not broken up in unexpected (or undesirable) locations.

8.18b Report Scheduling Violations Only After M&E Balances

When a scheduling violation is detected (e.g. equipment sharing violation) the application will report it right after the scheduling calculations are executed. The calculations normally are executed after:

1. the end of M&E balance calculations,
2. exiting an operation's i/o simulation dialog with **OK**,
3. exiting a procedure's data dialog with **OK**,
4. exiting an equipment's data dialog with **OK**,
5. exiting the process's scheduling information dialog with **OK**,
6. refreshing the contents of any scheduling chart (operations Gantt chart, equipment occupancy chart, etc.)

If you don't want to be bothered with the announcement of any scheduling conflicts after the closing of any of the dialogs mentioned above, then simply check this choice. You will only be notified of any scheduling conflicts after the conclusion of the M&E balance calculations.

8.18c Always Perform Section Yield Calculations

The yield calculations around each section, involve the mass flows and mass fractions of components on streams entering or exiting the section. If the M&E balances ended with errors or warnings there is a good chance that at least some of the yield calculations do not lead to valid fractions. Normally, SuperPro Designer will skip those calculations if errors and/or warnings were encountered during the execution of the M&E balances (for efficiency reasons). If you wish to have those values calculated regardless of the presence or absence of warnings/errors, then you should turn on the related preference.

8.18d Show Simulation Breakpoints

When placing a breakpoint in or around a unit procedure (see 8.15 Simulation Breakpoints), normally the application displays an indicator such as on if the breakpoint is active, or if the breakpoint is inactive. If you don't want the application to display such indicators, then you should turn this feature off.

8.18e Show Simulation Status Indicators for Each Procedure

When the simulation engine pauses after running into a simulation breakpoint, the application normally displays under every procedure an indicator to signify the status of the calculations in that procedure (e.g. a breakpoint in or around a unit procedure, normally the application displays an indicator such as to signify that all operations have been simulated successfully in that procedure, or if procedure has not been visited yet by the simulation engine (for more details, see 8.15 Simulation Breakpoints). If you don't want the application to display such indicators, then you should turn this feature off.

8.18f Update Simulation Status Indicators During M&E Balances

Normally, the application will not update the simulation (calculation) status of each procedure until the engine runs into a simulation breakpoint. If you wish to see the status indicators change dynamically (as the simulation progresses) then you should turn this feature on. Turning this feature on, along with the next ('Slow down simulation speed') may have the combined effect of visually following the sequence of solution as followed by the simulation engine.

8.18g Slow Down Simulation Speed

Sometimes it may be of interest to visually follow the solution sequence adopted by the simulation engine. Turning on this feature (along with the feature above, i.e. to 'Update Simulation Status Indicators During M&E Balances') will provide this feedback.

8.18h Apply External Auto-Initializations Upon Opening of Process File

Sometimes it is necessary to link the initialization of an input stream to the contents of another stream in another file (see 4.9 Auto-Initialization of Input Streams); similarly, instead of having equipment starting the simulation with contents simply be air, you may have designated the contents to be copied from the contents of another equipment in another file (see 6.1d Contents). If you turn on this feature, any such links get activated and executed right upon opening of the process file.

8.19 THE PROCESS FILE

When working on a process simulation many and diverse pieces of information need to be collected and integrated appropriately in order to produce a successful outcome. Raw materials (ingredients) need to be registered; unit procedures with their contained operations need to be created and initialized at the appropriate operating conditions; streams and their connectivity must be established to convey the transferring of material from one step to another; equipment (main and auxiliary) must be established that will host the processing steps; utilities in the form of heating and cooling agents must be introduced in order to accomplish any heating and/or cooling assignments; in the case of a batch simulation, the timing of all the actions must also be specified and recorded. Information on the participating elements in a process may originate from the System database, the User database or just be created for the purposes of the simulation case alone. All this information is kept in a process file. Besides the exact description of the process participants, a process file also contains the user's choices for many different aspects of the simulation cycle: the visual appearance of the graphical user interface, user's preferences for units in reports, charts, etc., just to name a few. All this information is kept inside the file and that is reason why these process files tend to grow very rapidly. By convention, all SuperPro Designer's files have the '.spf' extension, and all 'EnviroPro Designer' files have the '.epf' extension.

Just about every possible choice you can make while working with the application is either saved in your user profile (registry), see 8.20 Application Settings or it is already saved as part of your process file in order to facilitate your next change and/or adjustment to the process. The only piece of information that is NOT saved and cannot be customized to fit your preferences is the default values used to initialize the unit operations, main equipment resources or economic analysis and evaluation. These values are hard wired and may or may not be appropriate for your area of simulation. In a future version, users will be possible to create groups of settings that may be appropriate for their own industry (domain) and employ the appropriate set of defaults before starting a new simulation in that domain. To circumvent this limitation currently, see 8.19a Customizing Default Settings for a Domain of Applications

Since all the information related with a process is contained in a single file, keeping a safe copy of a process file is very important. Keeping backup copies of files on other media is also a good idea. To copy all the information contained in a process, all you have to do is copy a single file, the process file. You should also develop the habit of saving any incremental changes you have made to the process you are working on fairly often. In fact, an even better suggestion is to keep several versions of your process file, as it progresses from its inception stage to completion, under different file names. There are several compelling reasons for that. First, it allows you to review the evolutionary steps taken during the design of a process, and possibly revisit them later and entertain new options at any given phase of the design. Furthermore, it protects you against the possibility of a corrupted process file that could render all your work unreadable by the program. We have made every effort to eliminate all those unfortunate conditions that may corrupt a process file or lead a program to a crash, but as it is inevitably the case, there will always be some bugs that escape our testing. Some other times these situations might arise due to interactions with other programs running at that time on your machine, so it is impossible to predict. The best protection against such situations is to always be conservative and save several versions of your process file. Later in this chapter, we will propose a file system that allows you to keep all these versions organized within a project or across several projects.

8.19a Customizing Default Settings for a Domain of Applications

The current version of the software uses a single set of costing and economic evaluation factors derived from data that primarily apply to relatively large chemical and biochemical plants. The default factors may be substantially off for small plants that produce high value products or for very large bio/chemical plants that produce commodity products. To store your own factors for different types of plants, you might consider creating Seed (Template) Processes and use them as starting points whenever you wish to analyze a new process that resembles one of the template processes. To make sure that you can keep all these files around in an organized manner, you may consider following the paradigm proposed in the next section (see section 13.5). Future versions of SuperPro Designer will support generation of settings file for storing default values of multipliers and settings.

For cost analysis purposes, an alternative to setting files is to take advantage of the database capabilities of SuperPro Designer. Database sites store information on economic evaluation multipliers and other cost data and when a flowsheet section is allocated to a database site, it uses by default the factors of the site. Thus, a database site may function as a settings file. For more information on how to take advantage of the database capabilities for cost analysis, please consult the 'SynPharmDB' read-me file in the 'Examples \ SynPharm' directory of SuperPro Designer.

8.19b Working on a Long Term Project

As you probably need to have more than one alternative designs per project, and for each design, several revisions, this all adds up to many files. In order to keep all these files in an organized manner the scheme shown below

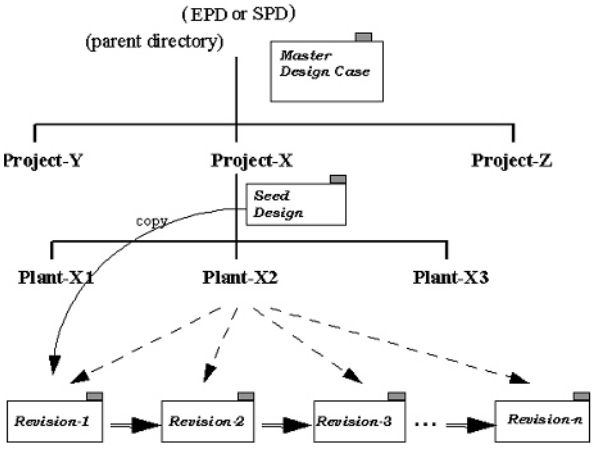


Figure 8.29: Organizing SuperPro Designer process files for a large project.

First of all, you need to keep all your files under a master subdirectory that bears the name of the software you are using (SuperPro Designer or EnviroPro Designer) and the version number. This is very important in case you later upgrade to a newer version or to SuperPro Designer, you need to keep the files separate. Under the master directory is a good place to keep your Master Process file. As you start a new project, you should create a new directory with a name bearing the name of the project. Chances are that you are going to be working on several projects and you definitely need to keep the files for each project separate. As you focus on a

specific project (e.g., Project-X), use that directory as the container of a Seed Process file. As you will probably have to deal with more than one alternative designs for each project (named 'Plant-X1', 'Plant-X2', etc. in the figure above), it is suggested that you create a separate subdirectory for each. You can start each alternative design by copying the entire seed process file into the corresponding subdirectory. Proceed by gradually adding the processing elements that compose your suggested configuration, making sure you save the design under several names (labeled 'Revision-1', 'Revision-2', etc. in the figure above) before you have added all the steps in your final revision. It is a good practice to keep ample comments as you progress from one revision to another documenting some of your decisions. Use the "Comments' field of the Flowsheet Attributes dialog, as the storage area for all such explanations.

8.19c Automatic Versioning (Archiving) of the Process File

The program, in an attempt to protect you against inadvertently losing your current process file, it automatically creates a set of backup (archive) files every time you save (**File ▸ Save** option from the main menu) any changes you made in your process and attempt to overwrite the previous version that already existed on the disk. The program will always maintain three versions for every process file:

1. Current (latest) Version: myfile.spf (for SuperPro) or myfile.epf (for EnviroPro)
2. Previously Saved Version: filename.sp~ or filename.ep~
3. Oldest Version: filename.s~~ or filename.e~~

Every time you save a process file by selecting **File ▸ Save** of the main menu or by clicking on the **Save** button ( ) or the **Save All** button ( ) of the main toolbar, all three files are updated: the oldest version is deleted, the previous version is renamed as filename.s~~ (or filename.e~~), the existing version is renamed as filename.sp~ (or filename.ep~) and finally the version you have just completed is saved under the filename.spf (or filename.epf) you have provided.

8.20 APPLICATION SETTINGS

Besides the properties that a process has on its own it also inherits some that are set in association with the application itself and of course, they apply to each of the documents (processes) created with it. Each of the following subsections deals with properties that apply to your preferences on how the application is run and are saved in your user profile (in the Windows Registry). All of the settings that are described in this section can be accessed and set from the Application Settings Dialog.

Since different users may be running this application under in the same PC, all the application preferences are saved under the particular user's profile. They will be enforced the next time the application is run by the same user, but they will have no effect on the appearance and behavior of the application when run by another user (on the same PC).

8.20a Announcements Upon Opening a Process File

Right after the application accesses the file where a process description is kept, it performs a few checks:

- *Format Compatibility Check*: First off, it makes sure that the process file format is compatible with the currently running application version and build number. Please remember that even though future versions of the application will be backwards compatible with previously created process files, the opposite is not the case. In other words, if a process file was created with an application version/build that is more recent than the running version/build, then the file will not open. Instead you will get an error message.
- *Resolution Mismatch Check*: Another check performed by the application is to verify if the resolution used when the process drawing was saved is the same as the current resolution (when you open the file). If not, then a necessary conversion is made. For a tips on how to deal with changing resolutions, see Screen Resolution.
- *DB-Site Consistency Check*: Another check made by the application upon opening a process file pertains only to files that contain mappings (allocations) to objects in the database. These objects (sites, equipment, heat transfer agents, labor, etc.) have values that are supposed to match exactly their database counterparts. As it is possible to edit the database objects independently of the process file that is being opened, it is conceivable that some of the contained object's database counterparts may have changed (in fact, some may no longer exist altogether!). If such a mismatch is detected, the application will notify you and prompt you to visit the Reconcile with Site DB Dialog.

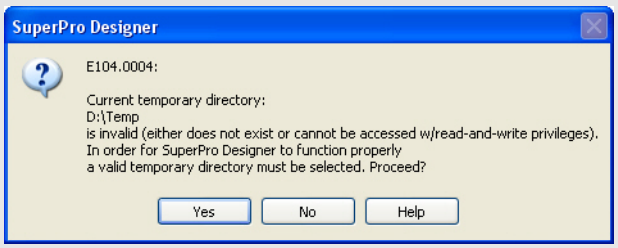
Since the application will always take a proper action (after the announcement is made) sometimes you may not want to see those announcements coming up after opening a file. This may be especially useful if you are using the COM interface of SuperPro Designer (see COM Library).

8.20b Automatic Background Saving of Modified Files

SuperPro Designer provides you protection against losing work due to a unexpected power failure or crash of the application. For as long as there are applications there will always be occasional crashes. Some of these crashes are such that the application can recover and continue to function normally. In these cases, no loss of data happens. However, if a more severe crash occurs, the application may be forced by the operating system to shut down immediately, without allowing the user to have a chance to save any open and modified files. This is where the auto-saving feature comes to the rescue. If the automatic saving is engaged (on) and say, set the auto-save interval to 15 minutes, you are guaranteed to never lose more than 15 minutes worth of work (should a crash occur). When the auto-save feature is on, SuperPro Designer will automatically save backups of all open files into a location under the designated temporary directory path. When the application is first installed the path is taken

from the 'TEMP' environment variable, but it can later be set to any folder that the user has read-and-write privileges.

If for whatever reason the designated temporary directory either no longer exists or it is no longer accessible from the user's running environment, the next time the application starts, it will complain and present the following message



*You must click **Yes** in the above message and then proceed to select a new, valid folder to be used as the application's temporary directory. If you don't, and click **No**, then the application will shut down.*

If you exit the application normally, all files created by the auto-save process are deleted. However, if a crash occurs, then the next time you start the application you will see a prompt notifying you that there are 'auto-saved versions' of files that are dated later than their corresponding last saved version (if any). If you choose to recover these files, then SuperPro Designer will automatically load up all these files for you to view and examine. You may choose later to keep by properly saving in a safe location or discard (i.e. close without saving) these files.

8.20c Temporary Directory Location

You must specify a directory (folder) on your PC (locally, not on a network drive) that the application can use to create temporary files (created during its normal operation - especially when generating reports) as well to save the automatically backed up files (see 8.20b Automatic Background Saving of Modified Files). Make sure that you have full read-and-write privileges in that location. If this folder becomes no longer accessible to the application (for reading and writing) then you will be warned and unless you pick a new valid folder, the application will not start.

Besides using the temporary directory for keeping backup files of your work-in-progress, the application also uses the temporary directory to create temporary files that are needed as part of the report generation process. If the application fails to complete a report successfully, it may leave some of those files behind (un-deleted). These files should be deleted the next time the application starts. If not, you may delete them manually at any time.

8.20d Startup Task

As soon as the application starts (after the startup billboards) it will present the Startup Task Dialog, questioning you what you wish to do as a startup task. This setting activates or deactivates this dialog from appearing during application startup. If you deactivate the dialog, then the last option chosen will be performed automatically (if possible). If you later wish to reactivate it and have the application present the Startup Dialog every time it boots up, you need set a flag from the Application Settings Dialog: Miscellaneous tab.

8.20e Batch Sheet Forms Folder

When generating the batch sheet for a batch recipe, there are many forms needed: for each operation type, for a procedure description, for component description, etc. All such forms are highly customizable and in case you have several versions of such forms kept in different folders, this selection tells the application where to look for those forms. For more details on the batch sheet, see Batch Sheet Generation.

8.20f Workspace Appearance

You can customize the appearance of the application in two basic areas:

(a) Choosing a Theme

(b) Handling of Multiple Open Process Files (Documents)

TABBED (WORKBOOK STYLE) VS. FLOATING VIEWS

SuperPro Designer provides a multi-document interface. In other words, you don't need to run multiple instances of the application in order to open multiple files. You can open as many process files as you want from a single running instance of the application. The choice in this box determines how you want to view and manage multiple workspaces (each corresponding to a different file).

(a) If you chose 'Tabbed'...

Each open file is shown in a window (workspace) that is automatically maximized to occupy all of the available space. When another file is opened, since it now occupies again all of the available space, it will complete overlap the previously open file.

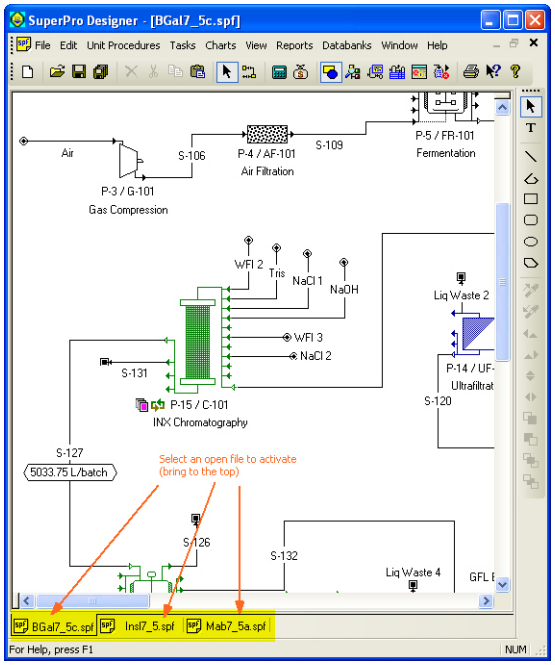


Figure 8.30: The 'tabbed' multi-document interface.

The previously opened files can be accessed by a tab shown at the bottom of the interface: Alternatively, the open files can be accessed by their distinct entry under the **Window** menu

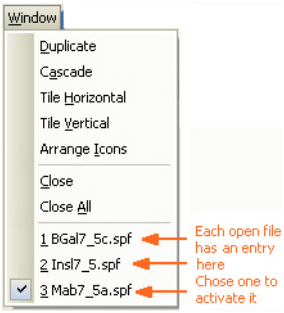


Figure 8.31: The Window menu (from the application's main menu).

(b) If you chose 'Floating'...

Each process file opened stays in its own workspace that can be sized at will and can be accessed and activated easily by clicking on it.

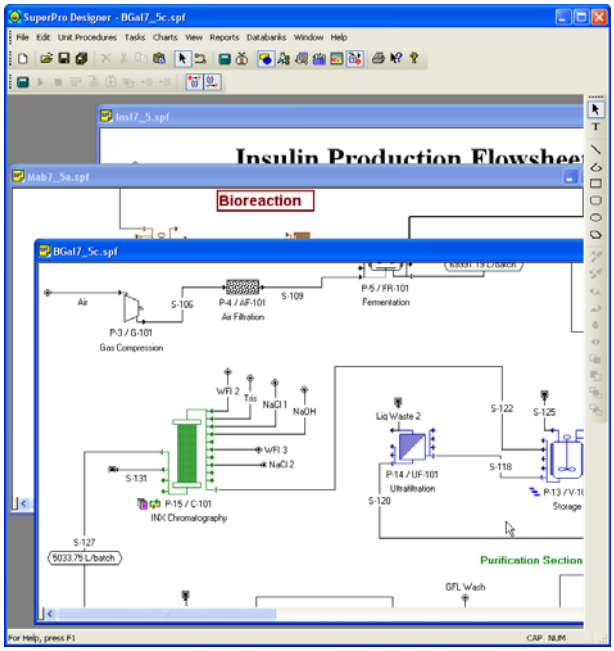


Figure 8.32: The 'floating' multi-document interface.

COLORING SCHEME

Starting with Windows XP, the operating scheme allows you to design (and install) your own personal preference for 'skins'. A skin determines the appearance of several visual elements of the operating system (such as window title bars, borders, background colors, etc.) The choices in the box, allow you to use such scheme (if available). Pick 'XP Skin' for this option. Alternatively, you may chose one of the other three (pre-defined) settings that we have selected for the application.

8.20g Database Access UserID & Password

Set the username that is to be used when SuperPro Designer accesses a user-editable database (e.g. the User DB, or the SchedulePro DB – if installed –). The userID may be required to keep track of changes in those databases and to provide you with proper privileges.

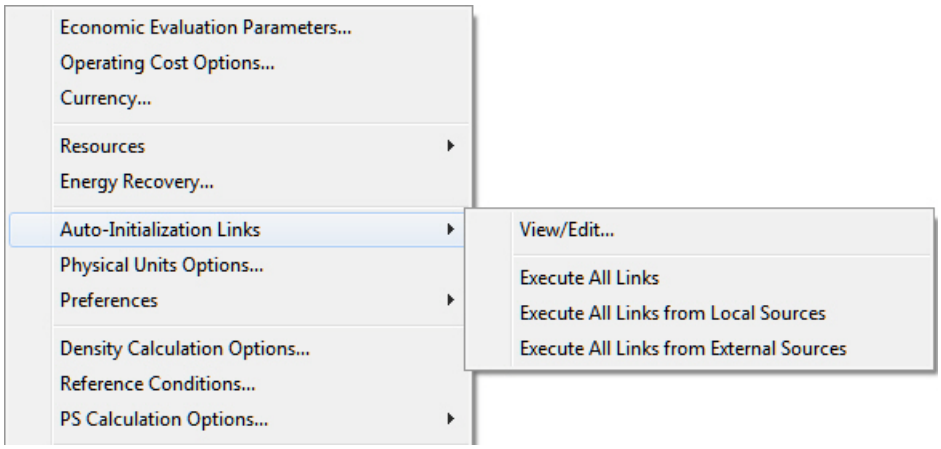
8.20h Automatic Name Generation

Every time you insert a new unit procedure in your process description (by selecting a unit procedure type from the **Procedures** menu and then clicking on the flowsheet or copying an existing procedure and then pasting it) the application must create a new unit procedure object and a new equipment resource to be used as the default host. Instead of always prompting you for names for the newly created objects, it uses a scheme to compose unique names for these objects. Of course users can later specify any name of their own choosing (see Edit Procedure Labels Dialog). The same principle applies when a new stream is created and attached to a unit procedure. Finally, when an operation is introduced in a unit procedure, once again, a name needs to be given so that it is unique within that procedure's sequence. In all those circumstances, the application composes a name by combining a core string (prefix) and a number. The prefix for creating streams is always the same (defaults to 'S-' for bulk streams and 'DS-' for discrete streams). The prefix for procedures is also fixed (irrespective of the procedure type) and it defaults to 'P-'. The prefixes used when naming equipment resources and operations depend on their types. For example, when creating the name for a chromatography column (of any type) 'C-' will be used (by default), whereas when creating the name for a fermentor, 'FR-' will be used. When creating a name for a charge operation 'CHARGE-' will be used whereas for a new filtration operation (of any type) 'FILTER-' will be used. The full name for all of the above objects is completed by appending a number to the prefix so that the entire name becomes unique. The default starting number for streams and equipment is '101' and for procedures is '1'. All of these settings (for prefixes and starting numbers) can be modified (if desired) to better suit your organization's (or even your own) expectations. Please note that just as is the case for all application settings discussed in this section, the new settings are saved as part of your own profile (in the Windows registry) and will be applied to all process files you work with.

8.21 AUTO-INITIALIZATION LINKS

The user may view and/or edit the auto-initialization links of input streams or equipment contents from a central location in SuperPro Designer. Right clicking on the flowsheet and selecting **Auto-Initialization Links ▸ View/Edit...** or will bring up the Auto-Initialization Links Dialog where one can view all the links that may exist in the current process, to the same file or to other files. From this interface the user may edit an Auto-Initialization link without

having the need to locate the specific input stream or unit procedure icon to do so.



From the **Auto-Initialization Links** menu seen above, the user can also:

(a) Execute the auto-initialization of all existing links in the file (local and external source links).

(b) Execute the auto-initialization only of links from local sources (same file).

(c) Or execute the auto-initialization only of links from external sources (other file).

1.

2.

Please note that it is important to apply the Temperature convergence option if the recycle loops contain operations such as Heat Exchangers, Evaporators or Condensers. These temperature dependant operations require energy balances around their unit procedure to be taken in account in order for the recycle loops to yield meaningful results.

9 ECONOMICS

An important feature of SuperPro Designer is that it facilitates the estimation of capital and operating costs and it also performs preliminary economic evaluation, profitability analysis and cash flow analysis of manufacturing and environmental processes. The key economic, financial, operating and market input parameters are analyzed by following common approaches that are available in the literature in order to determine four major economic aspects of an investment. These are:

- the total capital investment,
- the annual operating cost,
- the annual income, and
- the annual profits.

The analysis results are presented in the Executive Summary dialog and also in the form of three detailed reports: an Economic Evaluation Report (EER), an Itemized Cost Report (ICR), and a Cash Flow Analysis Report (CFR). Section 9.1 provides an overview of the steps involved in carrying out an economic analysis in SuperPro Designer. Sections 9.2 to 9.5 are dedicated to the description of the input parameters and calculations behind each of the four major economic variables. Section 9.7 describes the summary results and generated reports. Lastly, section 9.8 explains how to change the default currency used in a process model file.

9.1 OVERVIEW

Prior to performing economic calculations for a new project, some economic information must be first specified. Generally, the economic information considered in the calculations can be classified into the following categories:

1. *Material-related* information. This includes the different unit costs (e.g., purchase price, selling price, waste treatment/disposal cost) of pure components and stock mixtures.
2. *Stream-related* information. This includes the classification of input and output streams into different categories (e.g., raw materials, revenues, wastes, etc.).
3. *Operation-Related* information. This includes the unit costs of labor and utilities (heat transfer agents and power) for each operation.
4. *Equipment-related* information. This includes the capital and operating costs for each equipment (e.g., purchase cost, installation, maintenance, consumables, etc).
5. *Section-Related* information. This includes cost factors that are used to determine the capital and operating costs for each process section.

6. *Process-related* information. This includes economic evaluation parameters that are specified at the process level, such as time valuation, financing, production level and additional operating cost information for the entire project.

A key step in the economic calculations is the classification of streams into different categories and the specification of the costs associated with these streams. Each new stream added to a process flowsheet is initially unclassified. Therefore, *the specification of stream classification information must precede the economic evaluation calculations*. These can be specified through the Stream Classification Dialog which can be displayed by clicking **Stream Classification** on the **Tasks** menu.

Another important step in the calculations is the specification of the unit purchase cost, selling cost, and treatment or disposal cost of registered pure components and stock mixtures in a project. Default values are provided for a number of materials but some materials may have zero or outdated values. Similarly, default cost data and calculation options are provided for the bottom four economic information categories (e.g., unit costs of labor, power and consumables, equipment purchase cost, capital and operating cost factors with respect to purchase cost, information regarding time valuation, financing and production level, etc.). However, the default parameters may not be suitable for a particular project. Therefore, you are advised to examine the default economic parameters that are used in a project and make suitable changes where needed.

The economic calculations are performed by clicking **Perform Economic Calculations** () on the **Main** toolbar or on the **Tasks** menu. Note that the calculations of capital expenses, operating cost, income and profits are done around process sections. It is important to divide your process into a number of sections and take advantage of the cost breakdowns that pinpoint the cost-sensitive areas (the economic “hot-spots”) of a complex process.

The key analysis results are summarized in the ‘Executive Summary for Project’ dialog. To access this dialog, click **Executive Summary** on the **View** menu. In addition, the following reports can be generated:

- Economic Evaluation Report (EER): this report includes an executive summary that presents the key analysis results, a breakdown of the total capital cost, a breakdown of the annual operating cost and a description of profitability analysis calculations. To generate this report, click **Economic Evaluation (EER)** on the **Reports** menu.
- Cash Flow Analysis Report (CFR): This report includes loan information and detailed breakdowns of capital outlay, loan payment and cash flow for each year over the expected lifetime of a project. To generate this report, click **Cash Flow Analysis (CFR)** on the **Reports** menu.
- Itemized Cost Report (ICR): this report contains detailed cost breakdowns of the annual operating cost of all sections. This includes all cost items that are calculated at the section level. Additional cost items that are calculated at the process level are not considered. To generate this report, click **Itemized Cost (ICR)** on the **Reports** menu.

9.2 TOTAL CAPITAL INVESTMENT

The Total Capital Investment refers to the fixed costs that are associated with a process. This is calculated as the sum of the following cost items over all sections of a process:

1. Direct Fixed Capital
2. Working Capital
3. Startup and Validation Cost
4. Up-Front R&D Cost
5. Up-Front Royalties

In addition, the Capital Investment Charged to This Project is determined. This corresponds to the fraction of Total Capital Investment which is considered in the economic analysis of a particular project. This is useful in situations of multi-product facilities, in which an entire section or certain equipment of a section may be utilized by multiple projects; for more details, see 9.2f Capital Investment Charged to This Project.

Here is where you can find these figures:

- Both figures (Total Capital Investment and Capital Investment Charged to This Project) are shown in the Executive Summary Dialog: Summary Tab and in Sections 1 (Executive Summary) and 10 (Profitability Analysis) of the Economic Evaluation Report (EER).
- The Total Capital Investment is also shown in the Executive Summary Dialog: Capital Investment Tab.
- The individual cost items that contribute to the Total Capital Investment are shown in the Executive Summary Dialog: Capital Investment Tab and in Section 10 (Profitability Analysis) of the Economic Evaluation Report (EER).

Note that the Section 10 (Profitability Analysis) of the Economic Evaluation Report (EER) is generated only if the revenues of a project are positive.

The individual cost items that contribute to the Total Capital Investment are described in detail below.

9.2a Direct Fixed Capital (DFC)

The DFC refers to the fixed assets of an investment, such as plant and equipment. It is calculated at the process section level as the sum of direct, indirect and miscellaneous costs that are associated with a plant" s capital investment. The direct costs include cost elements that are directly related to an investment, such as the cost of equipment, process piping, instrumentation, buildings, facilities, etc. The indirect costs include costs that are indirectly related to an investment, such as the costs of engineering and construction. Additional costs such as the contractor's fee and contingencies are included in miscellaneous costs.

By default, the DFC is estimated using cost correlations to estimate the purchase cost of all major process equipment and cost factors with respect to purchase cost to generate estimates for all other cost elements. The installation factors are equipment-specific, whereas all other factors are specified at the section level.

Here is where you can find DFC-related figures:

- The Equipment Purchase Cost and DFC are shown in the Executive Summary Dialog: Capital Investment Tab.
- The DFC is also shown in Section 10 (Profitability Analysis) of the Economic Evaluation Report (EER). Note that this section is generated only if the revenues of a project are positive.
- The individual cost items that contribute to the DFC are shown in Section 3 (Fixed Capital Estimate Summary) of the Economic Evaluation Report (EER). An example is shown in Figure 9.1.

FIXED CAPITAL ESTIMATE SUMMARY (2005 prices in $)

3A. Total Plant Direct Cost (TPDC) (physical cost)	
1. Equipment Purchase Cost	2,212,000
2. Installation	1,766,000
3. Process Piping	774,000
4. Instrumentation	885,000
5. Insulation	66,000
6. Electrical	221,000
7. Buildings	996,000
8. Yard Improvement	332,000
9. Auxiliary Facilities	885,000
TPDC	8,138,000
3B. Total Plant Indirect Cost (TPIC)	
10. Engineering	2,034,000
11. Construction	2,848,000
TPIC	4,883,000
3C. Total Plant Cost (TPC = TPDC+TPIC)	
TPC	13,020,000
3D. Contractor's Fee & Contingency (CFC)	
12. Contractor's Fee	651,000
13. Contingency	1,302,000
CFC = 12+13	1,953,000
3E. Direct Fixed Capital Cost (DFC = TPC+CFC)	
DFC	14,973,000

Figure 9.1: The 'Fixed Capital Estimate Summary' section of the Economic Evaluation Report (EER).

The individual cost items that contribute to the DFC and the available calculation options for the DFC are described in detail below.

TOTAL PLANT DIRECT COST (TPDC)

The Total Plant Direct Cost (TPDC) is the sum of the following direct cost items:

- **Equipment Purchase Cost (PC)**: this is the vendor's selling price of major equipment. It excludes items such as taxes, insurance, delivery and installation. It is also known as the *free-on-board (FOB)* cost. For a preliminary economic analysis, the purchase cost of equipment is typically estimated based on cost correlations. SuperPro Designer provides correlations for estimating the purchase cost of major listed (modeled) equipment. The user may also provide his/her own cost values or cost correlations for all listed (modeled) equipment; for more details on these options, see 'Purchase Cost of Listed Equipment' on page 9-8 below. In SuperPro Designer, PC is calculated at the section level. For each section, the user may also specify the purchase cost of unlisted (overlooked) equipment as a factor of the section's PC. Generally, a section's PC will be the sum of the purchase costs of listed and unlisted equipment for that section.
- **Installation**: this cost item refers to the in-place erection of equipment at the new plant site and includes the cost of foundations, slabs, supports, and local equipment services. For a preliminary economic analysis, the installation cost of listed (modeled) equipment can be estimated by multiplying the corresponding purchase cost by a suitable factor; for more details, see 'Installation Cost of Listed equipment' on page 9-9. In SuperPro Designer, the installation cost is calculated at the section level. For each section, the user may also specify the installation cost of unlisted (overlooked) equipment as a factor of the corresponding purchase cost of unlisted equipment for that section. Generally, a section's installation cost will be the sum of the installation costs of listed and unlisted equipment for that section.
- **Process Piping**: this cost item incorporates the cost of process fluid piping that connects the equipment, as well as connections to the main utility headers and vents. Included are valves, piping supports, insulation, and other items associated with equipment piping. For a preliminary economic analysis, this cost is typically estimated by multiplying PC by a suitable factor. In SuperPro Designer, this cost is calculated at the section level as a factor of the section's PC.
- **Instrumentation**: this cost item includes the costs of transmitters and controllers (with all required wiring and tubing for installation), field and control room terminal panels, alarms and enunciators, indicating instruments both in the field and in the control room, on-stream analyzers, control computers and local data-processing units, and control room display graphics. For a preliminary economic analysis, this cost is typically estimated by multiplying PC by a suitable factor. In SuperPro Designer, this cost is calculated at the section level as a factor of the section's PC.
- **Insulation**: this cost item includes the cost of insulation and painting, which is usually included in the cost of installation and piping. In low temperature plants, however, insulation cost can become unusually high. An insulation surcharge is recommended for such plants. For a preliminary economic analysis, this cost is typically estimated by multiplying PC by a suitable factor. In SuperPro Designer, this cost is calculated at the section level as a factor of the section's PC.
- **Electrical**: this cost item refers to the cost of electrical facilities. These includes battery limits substations and transmission lines, motor switch gear and control centers, emergency power supplies, wiring and conduit, bus bars, and area lighting. Separate equipment estimation is required for electrolytic installations. For a preliminary economic analysis, this

cost is typically estimated by multiplying PC by a suitable factor. In SuperPro Designer, this cost is calculated at the section level as a factor of the section's PC.

- **Buildings**: this cost item includes the cost of process towers, subsidiary concrete slabs, stairways and catwalks (not equipment-specific), control rooms and other battery limits buildings (e.g., change rooms, cafeteria, furnished offices, warehouses, etc.). It also incorporates the costs for non-electric building services as well as for a variety of safety-related items. For a preliminary economic analysis, this cost is typically estimated by multiplying PC by a suitable factor. In SuperPro Designer, this cost is calculated at the section level as a factor of the section's PC.
- **Yard Improvement**: this cost item refers to the costs of excavation, site grading, roads, fences, railroad spur lines, fire hydrants, parking spaces, and others. For a preliminary economic analysis, this cost is typically estimated by multiplying PC by a suitable factor. In SuperPro Designer, this cost is calculated at the section level as a factor of the section's PC.
- **Auxiliary Facilities**: this cost item includes the cost of satellite process-oriented service facilities that are vital to the proper operation of the battery limits plant. An example of an auxiliary facility is a steam plant. For a preliminary economic analysis, this cost is typically estimated by multiplying PC by a suitable factor. In SuperPro Designer, this cost is calculated at the section level as a factor of the section's PC.

TOTAL PLANT INDIRECT COST (TPIC)

The Total Plant Indirect Cost (TPIC) is the sum of the following indirect cost items:

- **Engineering**: this cost item includes the preparation of design books that document the whole process (e.g., the design of equipment, specification sheets for equipment, instruments, auxiliaries, etc., the design of control logic and computer software, the preparation of drawings) and other engineering-related costs. For a preliminary economic analysis, this cost is typically estimated by multiplying TPDC by a suitable factor. In SuperPro Designer, this cost is calculated at the section level as a factor of the section's total direct cost.
- **Construction**: this cost item includes the costs associated with the organization of the total construction effort. They do not include the cost of construction labor. This is incorporated in direct cost items that involve construction. For a preliminary economic analysis, this cost is typically estimated by multiplying TPDC by a suitable factor. In SuperPro Designer, this cost is calculated at the section level as a factor of the section's total direct cost.

The sum of TPDC and TPIC is denoted as Total Plant Cost (TPC).

CONTRACTOR'S FEE AND CONTINGENCY COSTS (CFC)

The following additional costs are also considered:

- **Contractor's Fee**: this is the contractor's profit. It should be added even if a corporation does its own construction, because the construction division is expected to show a profit. For a preliminary economic analysis, this cost is typically estimated by multiplying TPC by a suitable factor. In SuperPro Designer, this cost is calculated at the section level as a factor of the section's total direct and indirect costs.
- **Contingency**: the more speculative a process is, the more likely it is that key elements have been overlooked during the project's early stages. This cost attempts to compensate for

missing elements. However, even advanced-stage estimates will include a contingency to account for unexpected problems during construction, such as strikes, delays, and unusually high price fluctuations. For a preliminary economic analysis, this cost is typically estimated by multiplying TPC by a suitable factor. In SuperPro Designer, this cost is calculated at the section level as a factor of the section's total direct and indirect costs.

Based on the above definitions, the total DFC of an investment is calculated as the sum of TPC and CFC.

ESTIMATION OF DFC

In SuperPro Designer, the DFC is estimated at the section level. Different options and parameters can be specified through a section's Capital Investment Dialog: DFC Tab. To access the 'Capital Investment' dialog for a process section, first select the desired section in the 'Section Name' drop-down list box that is available on the 'Section' toolbar. Then, do one of the following:

- click **Section Capital Cost Adjustments** ( ) on the same toolbar, or
- click **Process Options ▸ Section: <section name> ▸ Capital Cost Adjustments** on the **Edit** menu, or
- right-click on the flowsheet to bring up its context menu and click **Section: <section name> ▸ Capital Cost Adjustments**.

Note that the term in brackets represents the name of the selected section. The DFC of a section can be either:

- set by user, or
- estimated by multiplying the section's PC by a suitable 'composite' PC factor, or
- estimated as the sum of direct, indirect and other costs based on a distributed set of PC factors for the individual cost elements that contribute to these costs.

By default, a section's DFC is estimated based on the third option. If the second or the third option is selected, the section's PC must be first estimated. This is calculated as the sum of the total purchase costs of listed and unlisted equipment for that section. The total purchase cost of listed equipment for that section is calculated as the sum of individual purchase costs of all equipment present in that section. By default, the purchase cost of listed equipment is calculated using built-in cost correlations; for more details, see 'Purchase Cost of Listed Equipment' on page 9-8. The total purchase cost of unlisted equipment for that section is specified as factor of the section's PC.

If the DFC is estimated based on the third option, then additional cost items that contribute to the DFC are estimated. Similarly to the section's PC, the section's installation cost is calculated as the sum of total installation costs of listed and unlisted equipment for that section. The total installation cost of listed equipment for that section is calculated as the sum of individual installation costs of all equipment present in that section. The installation cost of listed equipment is specified as a factor of the equipment's purchase cost; for more details, see 'Installation Cost of Listed equipment' on page 9-9. The total installation cost of unlisted equipment for that section is specified as factor of the total purchase cost of unlisted equipment

for that section. Additional cost items that contribute to the section's DFC are specified as factors of the section's PC.

SuperPro Designer *uses a default set of PC factors that primarily applies to relatively large chemical and biochemical plants. These may be substantially off for small plants that produce high added value products, or for very large plants that produce commodity products. In these cases, appropriate PC factors must be specified by the user.*

You may choose to use site data for the PC factors. You can store distinct sets of economic factors behind model database sites and allocate the site with the most appropriate factors to relevant sections within your recipes; for more details, see 15.13 Sites & Resources Databank. Alternatively, you may save the economic factors of different types of plants into different files and use those files as starting points (like templates) whenever you wish to analyze a new process with similar economic characteristics.

Below, the calculation of the purchase and installation costs of listed equipment are described in detail.

PURCHASE COST OF LISTED EQUIPMENT

The total purchase cost of a section's listed (modeled) equipment is calculated as the sum of the purchase costs of all equipment resources of that section.

An equipment resource may represent multiple equipment units. It may include:

- a number of units (N) that are operated in parallel (i.e., simultaneously)
- extra sets of parallel units (M) that are operated in staggered mode (i.e., out of phase)
- a number of standby units (K)

Consequently, an equipment may represent a total of N(1+M)+K units. These values are specified through different tabs of the equipment's simulation data dialog:

- The number of parallel units and the extra sets of staggered units are specified through the Equipment Data Dialog: Equipment tab.
- The number of standby units is specified through the Equipment Data Dialog: Adjustments Tab.

Note that in equipment 'Design Mode', the number of units that are operated in parallel is calculated as part of the simulation; for more details, see 6.1 Main Equipment. To access the simulation data dialog of a host equipment, right-click on a unit procedure to bring up its context menu and select **Equipment Data**.

The purchase cost of an equipment resource will be equal to the corresponding purchase cost of a single unit of that type times the total number of units that it represents. For batch processes, only a fraction of that cost will be charged to each section. This is calculated as the fraction of total batch time that the equipment is in use by procedures contained in that section. This time factor is calculated by the program as part of the simulation.

Different specification options are available for the purchase cost of a single unit. These can be found in the Equipment Data Dialog: Purchase Cost Tab. The purchase cost of a single unit can be either:

(a) set by the user, or

(b) estimated based on a built-in model, or

(c) estimated based on a user-defined model.

By default, the purchase cost of equipment is estimated based on built-in cost correlations according to the second option. SuperPro Designer provides correlations for estimating the purchase cost of all major listed equipment. If the third option is selected, custom cost correlations can be specified based on the following power law:

$$PC = C_0 \left(\frac{Q}{Q_0} \right)^{\alpha} \qquad \text{eq. (9.1)}$$

where:

- C_0 is the base cost,
- Q_0 is the base capacity, and
- α is the exponent of the power law.

You may break the whole capacity range into any number of intervals and specify a set of power law data for each interval. To account for the time value of money, you must also specify the reference year for which the cost is valid. If the purchase cost is set by user, you may also specify a reference year or let the cost be fixed (independent of the year of the analysis); for more details, see 6.1f Purchase Cost.

The purchase cost in the year of analysis is calculated based on built-in values of the Chemical Engineering Cost Index for the reference year and the year of analysis. For years for which the Chemical Engineering Cost Index is not available, an inflation rate is used. The year of analysis and the inflation rate can be specified through the Economic Evaluation Parameters Dialog: Time Valuation Tab. To display the 'Economic Evaluation Parameters for Entire Project' dialog, do one of the following:

- click **Process Options ▸ Economic Evaluation Parameters** on the **Edit** menu, or
- right-click on the flowsheet to bring up its context menu and click **Economic Evaluation Parameters**.

By default, the year of analysis for a new project is the present year and the inflation rate is 4%.

The number of units that are operated in parallel, the number of standby unit, the number of staggered units, the unit cost and the total cost of all equipment present in the process are listed in Section 2 (Major Equipment Specification and FOB Cost) of a project's EER.

INSTALLATION COST OF LISTED EQUIPMENT

The total installation cost of a section's listed (modeled) equipment is calculated as the sum of the installation costs of all equipment resources of that section. For batch processes, only a fraction of that cost will be charged to each section. This is calculated as the fraction of total batch time that the equipment is in use by procedures contained in that section. This time factor is calculated by the program as part of the simulation.

The installation cost of an equipment resource is specified as a factor of its purchase cost. SuperPro Designer provides default installation factors for all major listed equipment. The

installation factor of an equipment resource can be viewed or edited through the Equipment Data Dialog: Adjustments Tab.

9.2b Working Capital

The working capital represents tied-up funds required to operate the business. It includes the investment in raw materials, consumables, etc. In SuperPro Designer, the working capital is specified at the section level. For each section, this can be either:

- set by the user, or
- estimated as the sum of major operational costs covered for a certain operating period; these include the costs for labor, raw materials, utilities (i.e., heating/cooling agents and power), waste treatment, and miscellaneous costs.

If the second option is selected, the user specifies the number of days that labor, raw materials, utilities and waste treatment costs are covered. The cost per section of each of the above items is calculated by multiplying the specified number of days by the corresponding daily cost of that item; for more details on the unit costs of the above cost items, see 9.3 Operating Cost. In addition, the user may specify an amount of money that is attributed to miscellaneous costs. The working capital of a section is calculated as the sum of all the above cost items.

The specification options for the working capital of a section can be edited through the Capital Investment Dialog: Misc Tab.

9.2c Startup and Validation Cost

The startup and validation cost includes pre-opening, one-time expenditures incurred to prepare a new plant for operation. In SuperPro Designer, the startup and validation cost is specified at the section level. For each section, this can be either:

- set by the user, or
- estimated as a percentage of DFC.

You may choose to use site data for the percentage of DFC that corresponds to the startup and validation cost of a section. You can store distinct sets of these factors behind model database sites and allocate the site with the most appropriate factors to relevant sections within your recipes; for more details, see 15.13 Sites & Resources Databank.

The startup and validation cost may optionally be depreciated; for more details, see *9.3o Depreciation.*

The specification options for the startup and validation cost of a section can be edited through the Capital Investment Dialog: Misc Tab.

9.2d Up-Front R&D Cost

The up-front R&D cost accounts for the cost of research & development required before a product is manufactured. In SuperPro Designer, this is specified at the section level through the Capital Investment Dialog: Misc Tab.

9.2e Up-Front Royalties

The up-front royalties account for the payments made for use of assets, resources, patents, etc. prior to the initiation of a project. In SuperPro Designer, this cost is specified at the section level through the Capital Investment Dialog: Misc Tab.

9.2f Capital Investment Charged to This Project

For each section, you can modify the fraction of the DFC that is assigned to this project. This is useful in situations of multi-product facilities, in which an entire section or certain equipment of a section may be utilized by multiple projects. This cost allocation can be made either on a section-wide basis or on a equipment-by-equipment basis. In the latter case, the user specifies the fraction of an equipment's purchase cost in that section which is assigned to this project. This information can be specified through the Capital Investment Dialog: Cost Alloc Tab.

If the DFC of a section is set by user, then only the section-wide cost allocation option will be available for that section.

The Capital Investment Charged to This Project is determined based on the cost allocation specifications for each section. It is calculated similarly to the Total Capital Investment except that it accounts only for the fraction of DFC that is assigned to this project. Its value is listed in the Executive Summary Dialog: Summary Tab and also in Sections 1 (Executive Summary) and 10 (Profitability Analysis) of the Economic Evaluation Report (EER). Note that the latter section is only available if the revenues of a project are positive.

9.3 OPERATING COST

The operating cost of a project includes costs that are related to the demand for a number of resources (i.e., raw materials, consumables, labor, heating/cooling utilities and power), as well as additional operational costs. More specifically, the annual operating cost (AOC) is calculated as the sum of the following cost items:

1. Materials cost
2. Consumables cost
3. Labor-dependent cost
4. Utilities (heating/cooling utilities and power) cost
5. Waste treatment/disposal cost
6. Facility-dependent cost
7. Laboratory/QC/QA cost
8. Transportation cost
9. Miscellaneous costs
10. Advertising/selling costs
11. Running royalties

12. Failed product disposal cost

If a project includes streams that are classified as credit, a net AOC is also calculated by subtracting the annual credits from the AOC; for more details, see 9.3p Net Annual Operating Cost. From the above cost items, the top nine cost items are calculated at the process section level. The bottom three cost items cannot be easily distributed to sections and are therefore calculated at the process level only.

Here is where you can find these figures:

- Both figures (AOC and net AOC) are shown in the Executive Summary Dialog: Summary Tab and in Sections 1 (Executive Summary) and 10 (Profitability Analysis) of the Economic Evaluation Report (EER).
- The AOC is also shown in the Executive Summary Dialog: Operating Cost Tab and in Section 9 (Annual Operating Cost) of the Economic Evaluation Report (EER).
- The individual cost items that contribute to the AOC are shown in the Executive Summary Dialog: Operating Cost Tab and in Section 9 (Annual Operating Cost) of the Economic Evaluation Report (EER).
- Detailed cost breakdowns of the fraction of the AOC that is calculated at the section level (consisting of the top nine cost items in the above list) are included in the Itemized Cost Report (ICR).

Note that the Section 10 (Profitability Analysis) of the Economic Evaluation Report (EER) is generated only if the revenues of a project are positive.

The individual cost items that contribute to the AOC are described in detail below.

9.3a Materials Cost

This is the total cost of all bulk materials (pure components and stock mixtures) and discrete entities that are utilized as raw materials in a process. These may include:

- bulk materials and/or discrete entities contained in process input streams that are either classified as ‘raw material’ or ‘cleaning agent’ streams, and
- bulk materials that are used as heat transfer agents in process operations.

The annual cost of each material is calculated by multiplying the corresponding unit cost (i.e., purchasing price) by the corresponding annual amount that is utilized in a process. The user specifies the unit costs of materials, whereas the corresponding annual amounts are calculated by the program as part of the simulation.

Here is where you can find these figures:

- The annual materials cost is shown in the Executive Summary Dialog: Operating Cost Tab and in Section 5 (Materials Cost) of the Economic Evaluation Report (EER).
- The unit cost, annual amount, and annual cost of individual raw materials are listed in Section 5 (Materials Cost) of the Economic Evaluation Report (EER).
- Detailed cost breakdowns of the annual materials cost are included in Section 4 (Material Cost) of the Itemized Cost Report (ICR).

Below, the specification options that are related to materials consumed in process input streams and for the manufacture of process heat transfer agents are described.

RAW MATERIAL AND CLEANING AGENT STREAMS

Process input streams can be classified as 'raw material' or 'cleaning agent' streams through the Stream Classification Dialog; for more details, see 4.10 Classification of Input and Output Streams.

The purchasing price of registered pure components can be specified through the Pure Component Properties Dialog: Economics Tab. To access this dialog, click **Pure Components ▸ Register, Edit/View Properties** on the **Tasks** menu and double-click on a component from the list of registered pure components; for more details on pure components, see 3.1 Pure Components.

The purchasing price of registered stock mixtures can be specified through the Stock Mixture Properties Dialog: Economics Tab. To access this dialog, click **Stock Mixtures ▸ Register, Edit/View Properties** on the **Tasks** menu and double-click on a mixture from the list of registered mixtures; for more details on stock mixtures, see 3.2 Stock Mixtures.

The purchasing price of discrete entities contained in discrete 'raw material' or 'cleaning agent' streams can be specified through the Discrete Input Stream Dialog: Entity Tab. To access this dialog, double-click on the corresponding stream; for more details on discrete streams, see 4.8 Discrete Streams.

HEAT TRANSFER AGENTS

The annual cost of a heat transfer agent may include a lumped cost that is included in the Utilities cost category and a material-based cost that is include in the Materials cost category. The material-based cost is calculated based on the annual amount and unit cost of the associated bulk material that is consumed for producing that agent; for more details, see 9.3m Cost of Heat Transfer Agents.

9.3b Consumables Cost

Some equipment require the use of at least one consumable. For example, a chromatography column requires the use of a resin. This cost element includes the costs of periodically replaced materials, such as membranes, chromatography resins, activated carbon, and other materials which may be required for the operation of process equipment. The annual cost of a consumable type utilized by an equipment unit is calculated by multiplying the corresponding unit cost (expressed as purchase cost per consumable amount) by the corresponding annual amount consumed:

$$\text{Annual Cost} = \text{Unit Cost} \times \text{Annual Amount} \qquad \text{eq. (9.2)}$$

The annual amount consumed is calculated by multiplying the consumable amount per use by the annual number of replacements:

$$\text{Annual Amount} = \text{Amount Per Use} \times \text{Annual Replacements} \qquad \text{eq. (9.3)}$$

The consumable amount per use is calculated by the multiplying the consumption rate (expressed as consumable amount per consumption basis) by the consumption basis (number of equipment unit or equipment size):

$$\text{Amount Per Use} = \text{Consumption Rate} \times \text{Consumption Basis} \qquad \text{eq. (9.4)}$$

Finally, the annual number of replacements is calculated by multiplying the consumable life (or replacement frequency) expressed per operating basis (operating cycles or hours) by the equipment's annual operating basis:

$$\text{Annual Replacements} = \text{Replacement Frequency} \times \text{Annual Operating Basis} \qquad \text{eq. (9.5)}$$

The user specifies the purchase cost, consumption rate (per consumption basis), and replacement frequency (per operating basis). The annual amount and cost of consumables are calculated by the program as part of the simulation.

Here is where you can find these figures:

- The annual consumables cost is shown in the Executive Summary Dialog: Operating Cost Tab and in Section 6 (Various Consumables Cost) of the Economic Evaluation Report (EER).
- The unit cost, annual amount, and annual cost of individual raw materials are listed in Section 6 (Various Consumables Cost) of the Economic Evaluation Report (EER).
- Detailed cost breakdowns of the annual consumables cost are included in Section 6 (Consumables Cost) of the Itemized Cost Report (ICR).

Existing consumables of the Consumables Databank can be added to equipment through the Equipment Data Dialog: Consumables Tab. Through the same dialog, the consumption rate and replacement frequency can be specified for each consumable; for more details, see 6.1h Consumables.

The purchase cost and life (replacement frequency) of consumables can be viewed (for the 'Designer' database) or edited (for the 'User' database) through the Consumables Properties Dialog: Identification tab. For consumables that are currently used in a process, these properties can be edited through the Consumables Currently Used by the Process Dialog dialog. To display the 'Consumables Currently In Use' dialog, do one of the following:

- click **Process Options ▸ Resources ▸ Consumables** on the **Edit** menu, or
- right-click on the flowsheet to bring up its context menu and click **Resources ▸ Consumables**.

To edit the properties of a consumable, double-click on the corresponding item on the list; for more details, see 6.1h Consumables.

Note that new consumables can be created and added to Consumables databank of the 'User' database. To access the 'Consumables Databank' dialog, click **Consumables** on the **Databanks** menu. To edit the properties of a user-defined consumable, click on a consumable type from the list on the left pane and then double-click on a consumable of that type from the list on the right pane, see 15.10 Consumables Databank.

9.3c Labor-Dependent Cost

This cost includes all labor-dependent operating costs except those for laboratory analyses, quality control and quality analyses, which is included in the Laboratory/QC/QA cost. In SuperPro Designer, the labor-dependent cost is calculated at the section level. More specifically, a total labor cost (TLC) is calculated for each section as the sum of the labor costs of the different labor types (i.e., operator, supervisor) that may be required for that section. The labor cost of each labor type is calculated by multiplying the corresponding labor demand per type (LDT) by the corresponding labor rate (i.e., unit cost) per type (LRT). For each section, the LDT may include:

- an itemized estimate (operating labor as defined in the process on a step-by-step basis), and
- a lumped estimate (additional labor defined on a lumped-time basis).

By default, only the itemized estimate is considered. For each labor type, the itemized estimate is calculated as the sum of individual labor demands by all operations of that section. Existing labor types of the Labor Types Databank can be added to operations through the Operations Dialog: Labor, etc Tab of an operation's simulation data dialog. To access this dialog, right-click on a unit procedure to bring up its context menu and then click **Operation Data**. Through the same dialog, an estimate of direct labor demand (effective work time devoted to process-related activities expressed in labor-hours per operating cycle or per operating hour) can be specified for each added labor type. The actual (total) labor demand is calculated by dividing the direct demand by the direct time utilization factor of that labor type; for more details, see 5.11a The Labor Etc. Group of Variables.

For each labor type, the lumped estimate is specified by the user. This information and the calculation options for the LDT of a section can be specified through the section's Operating Cost Adjustments Dialog: Labor Tab. To access the 'Operating Cost Adjustments' dialog for a process section, first select the desired section in the 'Section Name' drop-down list box that is available on the 'Section' toolbar. Then, do one of the following:

- click **Section Operating Cost Adjustments** ( ) on the same toolbar, or
- click **Process Options ▸ Section: <section name> ▸ Operating Cost Adjustments** on the **Edit** menu, or
- right-click on the flowsheet to bring up its context menu and click **Section: <section name> ▸ Operating Cost Adjustments**.

Note that the term in brackets represents the name of the selected section.

In the Operating Cost Adjustments Dialog: Labor Tab, the user may select among two different options for the calculation of the LRT of a section. This can be calculated using either:

- lumped labor rate estimates for all labor types, or
- detailed labor rate estimates for all labor types.

By default, the second option is selected. For each labor type, a detailed labor rate is estimated by adjusting the basic rate (i.e., the basic unit labor cost) for the following additional costs:

- **Fringe Benefits**: this refers to expenditures that are paid out by the company to cover various benefits which are not included in the basic labor rate.

- **Supervision**: this refers to the salaries of non-operational staff engaged in supervision of operational and clerical staff.
- **Operating Supplies**: this includes everyday items required to keep the plant in proper running condition, as well as clothing, tools, and protective devices for operators.
- **Administration**: this refers to the cost of non-process-related administrative and secretarial support.

The above costs are specified as factors of the basic rate. The detailed labor rate of a labor type is estimated as:

$$\begin{pmatrix}\text{Detailed}\\ \text{Labor Rate}\end{pmatrix} = \begin{pmatrix}\text{Basic}\\ \text{Rate}\end{pmatrix} \times \begin{pmatrix}1 + \text{Benefits} + \text{Supervision} +\\ \text{Supplies} + \text{Administration}\end{pmatrix} \qquad \text{eq. (9.6)}$$

The lumped rate, basic rate, basic rate adjustment factors and direct time utilization factors (for batch and continuous processes) of a labor type can be specified through the Labor Type Properties Dialog: Properties Tab. For labor types that are currently used in a process, these properties can be accessed through the List of Labor Types Currently Used by the Process dialog. To display the List of Labor Types Currently Used by the Process dialog, do one of the following:

- click **Process Options ▸ Resources ▸ Labor Types** on the **Edit** menu, or
- right-click on the flowsheet to bring up its context menu and click **Resources ▸ Labor Types**.

To edit the properties of a labor type, double-click on the corresponding item on the list. Note that by default, the 'Operator' type is always included in that list, regardless of whether it is actually used in the current process or not; for more details, see 6.11 Labor.

Note that new labor types can be created and added to labor types databank of the 'User' database. To access the 'Labor Types Databank' dialog, click **Labor Types** on the **Databanks** menu. To edit the properties of a user-defined labor type, switch to the 'User' database and double-click the desired item on the list; for more details, see 15.9 Labor Types Databank.

You may choose to use site labor types in a process section. You can store labor types with distinct properties behind model database sites and allocate the site with the most appropriate labor types to the relevant section(s) within your recipe; for more details, see Sites & Resources Databank.

Here is where you can find labor-related figures:

- The annual labor-dependent cost is shown in the Executive Summary Dialog: Operating Cost Tab and in Section 4 (Labor Cost) of the Economic Evaluation Report (EER).
- The unit cost, annual amount, and annual cost of individual labor types are listed in Section 4 (Labor Cost) of the Economic Evaluation Report (EER).
- Detailed cost breakdowns of the annual labor-dependent cost are included in Section 5 (Labor Cost) of the Itemized Cost Report (ICR).

9.3d Utilities Cost

This is the total cost of heating/cooling utilities (i.e., heat transfer agents) and power utilized in a process. It is the sum of the following costs:

- the cost of heat transfer agents utilized in every process operation,
- the cost of power utilized in every process operation, and
- the cost of additional power that may be required for each section; this includes the power consumption for unlisted equipment, support operations (e.g., night lighting), or other purposes that are not directly associated with the execution of any specific operation.

Note that there are two kinds of utilities (heat transfer agents and power) associated with an operation:

- utilities that are essential for an operation model (e.g., the heating/cooling required to achieve a temperature specification of a stream, or the power required to drive an equipment); these are specified either through the 'Oper. Cond's' tab or through the 'Utilities' tab of an operation's simulation data dialog; and
- a*uxiliary* utilities that may be optionally specified for an operation; these are specified through the Operations Dialog: Labor, etc Tab of an operation's simulation data dialog.

For essential utilities, the mass flow rate of a heat transfer agent and the power consumption of a power type can be either set or calculated as part of the simulation. For auxiliary utilities, these are always set by the user. The user also specifies the unit costs of heat transfer agents and/or power types utilized in a process and the amounts of additional power that may be required for each section.

The annual amount and cost of each utility are calculated by the program as part of the simulation. Here is where you can find these figures:

- The annual utilities cost is shown in the Executive Summary Dialog: Operating Cost Tab and in Section 8 (Utilities Cost) of the Economic Evaluation Report (EER).
- The annual amount and cost of individual utilities are listed in Section 8 (Utilities Cost) of the Economic Evaluation Report (EER).
- Detailed cost breakdowns of the annual utilities cost are included in Section 8 (Utilities Cost) of the Itemized Cost Report (ICR).

Below, the input data considered in the calculation of a section's utilities cost are described in detail.

HEAT TRANSFER AGENTS

The annual cost of a heat transfer agent may include a lumped cost that is included in the Utilities cost category and a material-based cost that is include in the Materials cost category. The lumped cost is calculated based on the annual amount of that agent and a lumped unit cost specified for that agent (either on a mass or energy basis); for more details, see 9.3m Cost of Heat Transfer Agents.

POWER TYPES

The annual cost of a power type consumed by process operations is calculated based on the annual amount and purchasing price of that power type. The purchasing price of a power type can be specified through the Power Type Properties Dialog: Properties tab. For power types that are currently used in a process, this property can be accessed through the List of Power Types Currently Consumed by the Process dialog. To display the 'Power Resources Currently Consumed' dialog, do one of the following:

- click **Process Options ▸ Resources ▸ Power Types** (or **Power Types Consumed**) on the **Edit** menu, or
- right-click on the flowsheet to bring up its context menu and click **Resources ▸ Power Types** (or **Power Types Consumed**)

To edit the properties of a power type, double-click on the corresponding item on the list; for more details, see 6.9 Power.

Note that new power types can be created and added to power types databank of the 'User' database. To access the 'Power Types Databank' dialog, click **Power Types** on the **Databanks** menu. To edit the properties of a user-defined power type, switch to the 'User' database and double-click the desired item on the list; for more details, see 15.8 Power Types Databank.

You may choose to use site power types in a process section. You can store power types with distinct properties behind model database sites and allocate the site with the most appropriate power types to the relevant section(s) within your recipe; for more details, see 15.13 Sites & Resources Databank.

ADDITIONAL POWER SPECIFICATIONS

For each section, an itemized estimate of electricity consumption is calculated as the sum of essential and auxiliary power consumption over all operations in that section. The user may specify the following additional power requirements for a section through a section's Operating Cost Adjustments Dialog: Utilities Tab:

- an amount of additional electricity demand (per year or per batch) for a selected power type,
- an additional general load demand (expressed as a percentage of total demand) for a selected power type, and
- an additional electrical power demand (expressed as a percentage of total demand) for a selected power type to account for unlisted (overlooked) equipment.

Therefore, a lumped estimate of additional electricity consumption is calculated by summing up the above contributions. The total electricity consumption of a section is the sum of the itemized and lumped estimates for that section.

9.3e Waste Treatment/Disposal Cost

This includes the cost of treatment or disposal of certain process output streams that correspond to wastes (e.g., undesirable by-products, solvents, etc.). Wastes are typically classified as solid, aqueous, organic, or gaseous (emissions). Depending on the phase, the complexity of the facility, and the nature of the waste, the treatment cost can vary substantially.

For a waste stream, you can either specify directly the unit cost of waste treatment/disposal, or allow it to be calculated based on the corresponding cost associated with each component present in that stream and the stream's composition. The annual amount and cost of each waste stream are calculated by the program as part of the simulation. The classification and treatment/disposal cost of waste streams can be specified through the Stream Classification Dialog; for more details, see 4.10 Classification of Input and Output Streams. The waste treatment/disposal cost of registered pure components is specified through the Pure Component Properties Dialog: Economics Tab; for more details on pure components, see 3.1 Pure Components.

The annual waste treatment/disposal cost for a project is shown in the Executive Summary Dialog: Operating Cost Tab. The unit cost, annual amount, and annual cost of treatment/disposal of waste streams are listed in Section 7 (Waste Treatment/Disposal Cost) of the Economic Evaluation Report (EER). In addition, detailed cost breakdowns of the annual waste treatment/disposal cost are included in Section 7 (Waste Cost) of the Itemized Cost Report (ICR).

9.3f Facility-Dependent Cost

This accounts for additional costs related to the use of a facility. In cases of new (green-field) designs, where no prior experience on the use of equipment exists, this is typically calculated as the sum of the costs associated with equipment maintenance, depreciation of the fixed capital cost, and miscellaneous costs such as insurance, local (property) taxes and possibly other overhead-type of factory expenses. For existing multi-product facilities, however, which are usually operated in batch, the estimation of maintenance- and depreciation-related expenses and the allocation of these expenses among different projects may not be straightforward. Therefore, it is usually more convenient for such facilities to calculate facility-related costs based on operating parameters. Optionally, in SuperPro Designer, both approaches can be used together. The annual facility-dependent cost for a project is shown in the Executive Summary Dialog: Operating Cost Tab and in Section 9 (Annual Operating Cost) of the Economic Evaluation Report (EER). In addition, detailed cost breakdowns of that cost are included in the Itemized Cost Report (ICR).

Generally, the facility-dependent cost of a section may include the following estimates:

- an estimate based on equipment usage/availability rates,
- an estimate based on a lumped facility availability rate,
- an estimate based on the production rate of the process, and
- an estimate based on capital investment parameters (i.e., maintenance, depreciation and miscellaneous costs).

The respective calculation options can be specified through the Operating Cost Adjustments Dialog: Facility Tab. By default, the third option is used. These options are described in detail below.

ESTIMATION BASED ON CAPITAL INVESTMENT PARAMETERS

This method will use the purchase cost of equipment as reference for computing (indirectly) the facility-dependent operating cost. This may include the following costs:

- maintenance,
- depreciation, and
- miscellaneous costs; these consist of insurance costs, local taxes and factory expenses.

Maintenance Cost

The maintenance cost accounts for the maintenance of the equipment and the facility in general. It can be estimated either:

- using equipment-specific multipliers, or
- as a percentage of the section's DFC that is assigned to this project.

Note that if the section's DFC is set by user, the first option will not be available; for more details, see 9.2a Direct Fixed Capital (DFC).

If the DFC of a section is set by user, the maintenance cost of that section can only be estimated as a percentage of a section's DFC.

If the first option is selected, the maintenance cost is calculated as the sum of individual equipment maintenance costs. The maintenance cost of each equipment is calculated by multiplying its purchase cost (the fraction that is assigned to this project) by a suitable maintenance factor. This factor can be specified through the Equipment Data Dialog: Adjustments Tab. For equipment resources that are shared by multiple sections, the maintenance cost is distributed to the various sections based on time utilization. More specifically, the maintenance cost of an equipment that is allocated to a particular section is calculated by multiplying the total maintenance cost of that equipment by the fraction of total utilized time that this equipment is being utilized by unit procedures in that section. The latter is calculated by the program as part of the simulation.

Depreciation

Depreciation is an income tax deduction that represents a fixed capital loss which is mostly due to equipment wear out and obsolescence. For each section, SuperPro Designer depreciates the fraction of DFC that is assigned to this project and has not been depreciated already minus its salvage value at the end of the project lifetime. The user also has the option to depreciate the startup and validation cost. The annual depreciation of a section's assets, which contributes to the facility-dependent costs of a section, is calculated based on the straight-line method; for more details, see 9.3o Depreciation.

Miscellaneous Facility-Dependent Costs

Miscellaneous costs include the following individual costs:

- **Insurance**: insurance rates depend to a considerable extent upon the maintenance of a safe plant in good repair condition. The processing of flammable, explosive, or dangerously toxic materials usually results in higher insurance rates.
- **Local Taxes**: these refer to local property taxes (not income taxes).

- **Factory Expenses**: these refer to the overhead cost incurred by the operation of non-process-oriented facilities and organizations, such as accounting, payroll, fire protection, security, cafeteria, etc.

Each of the above cost items is specified as a percentage of the DFC.

You may choose to use site data for the miscellaneous facility-dependent costs of a process section. You can store distinct sets of these factors behind model database sites and allocate the site with the most appropriate factors to the relevant section(s) within your recipe; for more details, see 15.13 Sites & Resources Databank.

ESTIMATION BASED ON EQUIPMENT USAGE/AVAILABILITY RATES

This estimate of facility-dependent cost is calculated as the sum of individual equipment contributions to this cost. Each contribution may be viewed as a rental fee for the use of the corresponding equipment, which is calculated either:

- by multiplying the equipment usage rate (the costing rate based on usage) by the hours that the corresponding equipment is actually used by a section (usage basis), or
- by multiplying the equipment availability rate (the costing rate based on availability) by the hours that the corresponding equipment is reserved for a section (availability basis).

Optionally, the user may exclude some of the equipment utilized in the modeling (e.g. mixers, splitters, etc.) so that they do not artificially inflate the overall equipment usage- or availability-dependent cost. The usage and availability rates of an equipment can be specified through the Equipment Data Dialog: Adjustments Tab. The equipment usage and availability hours are calculated by the program as part of the simulation; for more details, see 6.1 Main Equipment.

ESTIMATION BASED ON FACILITY AVAILABILITY RATE

Instead of tallying up the equipment usage or availability hours for each equipment, one may utilize a flat rate for the entire facility. Using this approach, a facility-dependent cost is calculated by multiplying the specified facility availability rate by the hours that the facility is available. The latter are calculated by the program as part of the simulation.

You may choose to use site data for the facility availability rate of a process section. You can store distinct rates behind model database sites and allocate the site with the most appropriate rate to the relevant section(s) within your recipe; for more details, see 15.13 Sites & Resources Databank.

ESTIMATE BASED ON PRODUCTION RATE

The facility-dependent cost may also be estimated based on the unit production reference rate specified from the Main Product/Revenue stream and flow basis (see also Main Product/Revenue Rate) or from the unit rate reference flow. It is calculated by multiplying the specified unit cost by the unit production cost reference rate, which is calculated by the program during simulation.

9.3g Laboratory / QC / QA Cost

This accounts for the cost of off-line analysis, quality control (QC) and quality assurance (QA) costs. Chemical analysis and physical property characterization from raw materials to final

product is a vital part of chemical operations. In SuperPro Designer, this cost is estimated for each section. It may include:

- a lumped estimate calculated as a percentage of a section's total labor cost (TLC), and
- a detailed estimate calculated as the sum of the costs of different tests carried out and of a fixed cost for QA activities; in that case, the user specifies detailed information about the number and unit cost of the various assays along with a fixed cost for QA activities.

By default, this cost is calculated for each section based on the first option. The above options can be specified through the Operating Cost Adjustments Dialog: Lab/QC/QA Tab.

The total laboratory/QC/QA cost of a project is the sum of individual costs per section over all sections. The annual laboratory/QC/QA cost for a project is shown in the Executive Summary Dialog: Operating Cost Tab and in Section 9 (Annual Operating Cost) of the Economic Evaluation Report (EER). In addition, detailed cost breakdowns of that cost are included in the Itemized Cost Report (ICR).

9.3h Transportation Cost

This accounts for the cost of long-distance transportation of raw materials and products by sea, land, and air. Transportation operations are the only process steps that can contribute to transportation cost. The following operations are available:

- Transport by Truck (Bulk Flow)
- Transport by Truck (Discrete Flow)
- Transport by Train
- Transport by Sea
- Transport by Air

The primary objective of transportation operations is to account for and estimate the shipping cost associated with the transportation of raw materials and finished products of a manufacturing facility. Through the cost-related tab of a transportation operation's dialog, the user specifies the following cost factors:

- fixed cost (per shipment),
- quantity dependent cost (i.e., cost per shipping quantity), and
- quantity and distance dependent cost (i.e., cost per shipping quantity and shipping distance)

The annual transportation cost (ATC) is estimated using the following equation:

$$ATC = s_0 \left(C_0 + s_1 C_1 + s_1 s_2 C_2 \right) \qquad \text{eq. (9.7)}$$

where:

- s_0 is the number of shipments per year,
- C_0 is the fixed cost,
- s_1 is the quantity per shipment,

- C_1 is the quantity-dependent cost,
- s_2 is the shipping distance, and
- C_2 is the quantity- and distance-dependent cost.

For units that transport bulk material as well as discrete entities, the above equation is applied twice. The annual transportation cost for a project is shown in the Executive Summary Dialog: Operating Cost Tab and in Section 9 (Annual Operating Cost) of the Economic Evaluation Report (EER). In addition, detailed cost breakdowns of that cost are included in the Itemized Cost Report (ICR).

9.3i Miscellaneous Operating Costs

This cost element accounts for:

- on-going R&D expenses,
- process validation expenses, and
- other overhead-type expenses that are not covered by other cost categories.

By default, this cost item is zero. The relevant specification parameters can be modified through the Operating Cost Adjustments Dialog: Misc Tab. For each section, the process validation expenses are specified as a fixed cost (per year or per batch). Each of the on-going R&D and other expenses categories may include:

- a fixed cost term (per year or per batch), and
- a variable cost, which is specified as cost per kg of main product.

For the first term, the conversion between annual cost and cost per batch is based on the specified or calculated annual number of batches for this project; for more details, see 7.2c Recipe/Process-Level Scheduling Information. For the second term, an annual cost is calculated by multiplying the variable cost by the annual ‘Main Product/Revenue’ rate. Optionally, the ‘Main Product/Revenue’ rate may be discounted by the main product failure rate; for more details, see 9.3q Main Product/Revenue Rate. For each section, the annual miscellaneous costs are calculated as the sum of annual on-going R&D expenses, process validation expenses and other expenses. The total miscellaneous costs for the project are calculated as the sum of miscellaneous costs for each section over all sections.

The annual miscellaneous costs for a project are shown in the Executive Summary Dialog: Operating Cost Tab and in Section 9 (Annual Operating Cost) of the Economic Evaluation Report (EER). In addition, detailed cost breakdowns of these costs are included in the Itemized Cost Report (ICR).

9.3j Advertising and Selling Costs

This is the cost that is associated with the activities of the sales department. It may include:

- a fixed annual cost, and
- a variable cost, which is specified as cost per kg of main product.

These can be specified through the “Misc.” tab of the Economic Evaluation Parameters Dialog: Misc. Tab. Note that the default values for both cost terms are zero.

For the second term, an annual cost is calculated by multiplying the variable cost by the annual 'Main Product/Revenue' rate. Optionally, the 'Main Product/Revenue' rate may be discounted by the main product failure rate; for more details, see 9.3q Main Product/Revenue Rate.

The annual advertising and selling costs for a project shown in Section 9 (Annual Operating Cost) of the Economic Evaluation Report (EER). They are also included in the sum of advertising and selling, running royalty, and failed product disposal costs that is listed as 'Other Costs' in the Executive Summary Dialog: Operating Cost Tab.

9.3k Running Royalties

If the process, any part of the process, or any equipment used in the process are covered by a patent not assigned to the corporation undertaking the new project, permission to use the teachings of the patent must be negotiated, and some form of royalties is usually required. The licensing agreement usually calls for a flat charge per unit of product or else a percentage on the sales dollar.

In SuperPro Designer, the user specifies the running royalty expenses as cost per kg of main product. This is specified through the Economic Evaluation Parameters Dialog: Misc. Tab. Note that the default value for this cost is zero.

The annual running royalty expenses are determined by multiplying the specified cost by the annual 'Main Product/Revenue' rate. Optionally, the 'Main Product/Revenue' rate may be discounted by the main product failure rate; for more details, see 9.3q Main Product/Revenue Rate.

The annual running royalty expenses for a project are shown in Section 9 (Annual Operating Cost) of the Economic Evaluation Report (EER). They are also included in the sum of advertising and selling, running royalty, and failed product disposal costs that is listed as 'Other Costs' in the Executive Summary Dialog: Operating Cost Tab.

9.3l Failed Product Disposal Cost

This is the cost associated with the disposal or off-site recycling of scrapped product. In SuperPro Designer, the user specifies:

- the disposal cost per kg of main product scrapped, and
- the main product failure rate as percent of main product.

These can be specified through the Economic Evaluation Parameters Dialog: Production Level Tab. Note that the default values for these parameters are zero.

An annual failed product disposal cost is calculated by multiplying the corresponding disposal cost per kg of main product scrapped by the 'Main Product/Revenue' rate and the main product failure rate; for more details, see 9.3q Main Product/Revenue Rate.

The annual failed product disposal cost for a project is shown in Section 9 (Annual Operating Cost) of the Economic Evaluation Report (EER). It is also included in the sum of advertising and selling, running royalty, and failed product disposal costs that is listed as 'Other Costs' in the Executive Summary Dialog: Operating Cost Tab.

9.3m Cost of Heat Transfer Agents

The annual cost of a heat transfer agent may generally include:

- a lumped utility cost that is calculated based on the annual amount and lumped unit cost (specified either on a mass or energy basis) of that agent, and
- a material-based cost that is calculated based on the annual amount and unit cost of the associated bulk material that is consumed for producing that agent.

By default, the annual cost of a heat transfer agent includes only the lumped unit cost-based estimate. The corresponding cost is included in the Utilities Cost category; for more details, see 9.3d Utilities Cost. Optionally, a heat transfer agent may be associated with a registered pure component or stock mixture. In that case, a material-to-agent consumption factor may be specified for that agent. This will determine the fraction of the annual amount of that agent that corresponds to the annual amount of the associated bulk material that is consumed for producing that agent. The corresponding annual cost of the bulk material which is associated with the agent will be included in the Materials Cost category.

The annual cost of a heat transfer agent may consist of a lumped cost which is included in the Utilities cost category and a material-based cost which is included in the Materials cost category.

The lumped unit cost, the associated material and the material-to-agent consumption factor can be specified through the Heat Transfer Agent Properties Dialog: Properties tab. For heat transfer agents that are currently used in a process, these properties can be accessed through the List of Heat Transfer Agents Currently in Use dialog. To display the 'Heat Transfer Agents Currently In Use' dialog, do one of the following:

- click **Process Options ▸ Resources ▸ Heat Transfer Agents** on the **Edit** menu, or
- right-click on the flowsheet to bring up its context menu and click **Resources ▸ Heat Transfer Agents**.

To edit the properties of a heat transfer agent, double-click on the corresponding item on the list; for more details, see 6.7 Heat Transfer Agents.

Note that new heat transfer agents can be created and added to Heat Transfer Agents databank of the 'User' database. To access the 'Heat Transfer Agents Databank' dialog, click **Heat Transfer Agents** on the **Databanks** menu. To edit the properties of a user-defined heat transfer agent, switch to the 'User' database and double-click the desired item on the list; for more details, see 15.7 Heat Transfer Agents Databank.

You may choose to use site heat transfer agents in a process section. You can store agents with distinct properties behind model database sites and allocate the site with the most appropriate agents to the relevant section(s) within your recipe; for more details, see 15.13 Sites & Resources Databank.

9.3n Unit Production/Processing Cost

Upon determination of the annual operating cost (AOC) (see 9.3 Operating Cost), a unit production or processing cost can be calculated by dividing the AOC by a selected 'Unit Reference Rate'; for more details, see 9.3r Unit Reference Rate (or Flow). Depending on whether the 'Unit Reference' stream that is associated with the 'Unit Reference' rate is a process input or output stream, the corresponding unit cost is denoted as 'processing' or 'production', respectively.

The unit production/processing cost is shown in the Executive Summary Dialog: Summary Tab and in Sections 1 (Executive Summary) and 10 (Profitability Analysis) of the Economic Evaluation Report (EER). Note that the latter section is only available if at least one revenue stream with non-zero selling price or processing fee exists in the project.

9.3o Depreciation

Depreciation is an income tax deduction that represents a fixed capital loss which is mostly due to equipment wear out and obsolescence. It may be considered as a time-dependent operating cost, spread over a predefined depreciation period. For each section, SuperPro Designer depreciates the fraction of DFC that is assigned to this project and has not been depreciated already minus its salvage value at the end of the depreciation period. The user also has the option to depreciate the startup and validation cost. In the general case, the total depreciable amount, d_{tot}, of a section's assets over the entire depreciation period is calculated as:

$$d_{tot} = \sum_{1}^{N} d_k = B - S \qquad \text{eq. (9.8)}$$

where:

$$B = f_p \times UDFC + C_s \qquad \text{eq. (9.9)}$$

$$S = f_s \times f_p \times UDFC \qquad \text{eq. (9.10)}$$

and:

- d_k is the depreciable amount of a section's assets in year *k*,
- N is the depreciation (recovery) period,
- B is the cost basis of a section's assets (the cost right before the project starts)
- S is the salvage value of the section's assets at the end of the depreciation period,
- f_p is the fraction of a section's DFC that is assigned to this project,
- UDFC is the undepreciated DFC of a section (i.e., the fraction of a section's DFC that has not been depreciated already),
- C_s is the startup & validation cost of a section, and
- f_s is the salvage fraction of the entire DFC.

Three classical methods are available for the calculation of the annual depreciation of a section's assets, namely:

- the straight-line method,
- the declining balance method, and
- the sum-of-the-years-digit method.

The straight line method assumes a constant annual depreciation which is calculated for year *k* as follows:

$$d_k = d_{tot}/N \qquad \text{eq. (9.11)}$$

The declining balance method assumes a constant depreciation rate and, therefore, decreasing annual depreciable amounts. Based on this method, the annual depreciation for year *k* is calculated based on the following equations:

$$d_k = R \times (BV)_{k-1} \qquad \text{eq. (9.12)}$$

where:

$$(BV)_k = B(1-R)^k \qquad \text{eq. (9.13)}$$

$$R = 1 - f_s^{1/N} \qquad \text{eq. (9.14)}$$

and:

- R is the depreciation rate, and
- $(BV)_k$ is the book value (i.e., the amount that has not bee depreciated) of a section's assets in year *k*.

The sum-of-the years-digit method also assumes decreasing annual depreciable amounts. Based on this method, the annual depreciation for year *k* is calculated as:

$$d_k = N_k d_{tot}/SYD \qquad \text{eq. (9.15)}$$

$$N_k = N - k + 1 \qquad \text{eq. (9.16)}$$

$$SYD = N(N+1)/2 \qquad \text{eq. (9.17)}$$

where:

- N_k is the remaining depreciable life at the beginning of year *k*, and
- SYD is the sum-of-years digits.

Note that the annual depreciation of a section's assets, which contributes to section's facility-dependent costs, is calculated based on the straight-line method. All three depreciation methods are available for cash flow analysis calculations.

In the calculation of the annual operating cost, the depreciation term is calculated based on the straight-line method.

The undepreciated DFC of a section can be calculated either:

- based on the undepreciated purchase cost of equipment, or
- based on the specified percentage of a section's DFC assigned to this project that has already been depreciated.

Note that the first option is only available if the DFC is not set by the user; for more details, see 9.2a Direct Fixed Capital (DFC).

If the DFC of a section is set by user, the undepreciated DFC of a section can only be estimated based on the specified percentage of a section's DFC that has already been depreciated.

If this option is selected, the undepreciated DFC is calculated similarly to the DFC except that the purchase cost of listed equipment is now calculated as the sum of undepreciated equipment purchase costs. For each equipment, the undepreciated purchase cost is determined by subtracting the fraction of the purchase cost that has already been depreciated from the purchase cost. This fraction is specified through the Equipment Data Dialog: Adjustments Tab.

The fraction, f_p, of DFC that is assigned to this project is specified, either directly or on a unit-by-unit basis, through the section's Capital Investment Dialog: Cost Alloc Tab; for more details, see 9.2a Direct Fixed Capital (DFC).

The startup & validation cost and the option to depreciate this cost can be specified through the section's Capital Investment Dialog: Misc Tab; for more details, see 9.2c Startup and Validation Cost.

The calculation method for undepreciated DFC of a section and the option to depreciate this cost can be specified through the section's Operating Cost Adjustments Dialog: Facility Tab; for more details, see 9.3f Facility-Dependent Cost.

The method of depreciation (for cash flow analysis calculations), the salvage fraction, f_s, of DFC and the depreciation period, N, can be specified through the Economic Evaluation Parameters Dialog: Financing Tab. The default value for the salvage fraction is 5% of DFC and the default depreciation period is ten years.

The starting year of construction can be specified through the Economic Evaluation Parameters Dialog: Time Valuation Tab. The default starting year of construction is the present year.

9.3p Net Annual Operating Cost

If a project includes streams that are classified as credit or generated power that is recycled or heat that is recovered from operations, then a net annual operation cost (AOC) is calculated by subtracting these credits and/or savings from the AOC.

The value of the net AOC is shown in the Executive Summary Dialog: Summary Tab (if the annual credits are not zero) and in Sections 1 (Executive Summary) and 10 (Profitability Analysis) of the Economic Evaluation Report (EER).

For more details on the AOC, see 9.3 Operating Cost; for more details on credit streams, recycled power and recovered heat, see 9.4 Income.

9.3q Main Product/Revenue Rate

The 'Main Product/Revenue Rate' is a reference mass flow rate that corresponds to the stream that is specified as the 'Main Product/Revenue' stream. In case a process produces multiple 'Revenue' streams, a user may designate one as the 'Main Produce/Revenue' stream, as typically a production process is designed to manufacture a 'main' product that will be the main source of revenue, even though other side products may result and provide supplementary income. The user may specify a 'Main Product/Revenue' stream and an associated flow basis (total or component flow) through the Stream Classification Dialog dialog; for more details, see 4.10 Classification of Input and Output Streams.

This rate is used to convert a specified variable cost (e.g., cost per kg of main product) into annual cost. Variable costs can be specified for the following cost items:

- Miscellaneous Costs, see 9.3i Miscellaneous Operating Costs;
- Advertising and Selling Costs, see 9.3j Advertising and Selling Costs;
- Running Royalties, see 9.3k Running Royalties;
- Failed Product Disposal Cost, see 9.3l Failed Product Disposal Cost.

In the first three cases, an annual cost is calculated by multiplying the variable cost by the annual 'Main Product/Revenue' rate. Optionally, the 'Main Product/Revenue' rate may be discounted by the main product failure rate. This option can be specified through the Economic Evaluation Parameters Dialog: Production Level Tab. In this tab, the user may specify a main product failure rate and choose to apply this rate to all reference rates ('Main Product/Revenue', 'Unit Reference', and 'Throughput') by checking the option entitled 'Apply Failure Rate to All Reference Rates?'. If this option is checked, a discounted 'Main Product/Revenue' rate is calculated by multiplying the 'Main Product/Revenue' rate by (1 - 'Failure Rate'). If the failure rate is non-zero, then an annual failed product disposal cost is calculated by multiplying the amount of 'failed' product rate by a disposal cost (set by the user). For more details on the 'Main Product/Revenue Rate' and streamselection, see 'Main Product/Revenue Rate Stream' on page 4-29.

9.3r Unit Reference Rate (or Flow)

The 'Unit Reference Rate' (or Flow) is used to convert a calculated annual cost into a per-unit cost (e.g., cost per kg of raw materials or products). It corresponds to the total flow or a component flow in a selected 'Unit Reference Stream'. The 'Unit Reference Stream' and flow basis are specified through the Rate Reference Flows Dialog: Unit Reference tab. To display the 'Rate Reference Flows' dialog, click **Rate Reference Flow(s)** on the **Tasks** menu. If the 'Unit Reference Stream' is the same as the 'Main Product/Revenue Stream', the 'Unit Reference Rate' will correspond to the 'Main Product/Revenue Rate'. Optionally, the 'Main Product/Revenue Rate' may be discounted by the product failure rate; for more details, see 9.3q Main Product/Revenue Rate.

9.4 INCOME

The income of a project consists of all proceeds from plant operation. Typically, this refers to the revenues of a project. Optionally, for reporting purposes, part of the revenues may be specified as credits. These are not included in reported revenues. Instead, they are used to lower the reported (net) operating cost. The latter is calculated as the difference between the actual operating cost and credits. The two types of income (revenues and credits) are described in detail below.

9.4a Revenues

This consists of all revenues associated with the operation of a plant. These may include all proceeds from:

- the sale of main and side products,
- the processing of influent streams (for waste treatment and disposal plants), and
- the sale of generated electricity.

In SuperPro Designer, the first two revenue sources are determined based on the flow and unit price of streams that are specified as being 'revenue' streams. The last revenue source is determined based on the amount and unit price of generated power that is denoted as 'revenue'. These are described below in detail.

REVENUE STREAMS

Revenue streams are process input and/or output streams that contribute to the revenues of the project. For most manufacturing processes, revenue streams are typically process output streams (i.e., products). For waste treatment facilities, however, revenue streams could be process input streams that carry waste, if the proceeds from the operation of the plant are based on the amount of waste treated. Each revenue stream can have a unit *selling price* (if it is an output stream) or a unit *processing fee* (if it is an input stream) associated with it. This can either be calculated by the program based on the Selling Price of each component present in that stream and the stream's composition, or it can be set by the user.

In addition, a single revenue stream can be specified as the 'Main Product/Revenue' stream. This is the revenue stream which is considered as the main revenue source for the project. This distinction between the main revenue source and other revenue sources is used in the executive summary dialog and in the Economic Evaluation Report (EER). In addition, this stream may be used as reference for specifying a project's advertising/selling and running royalty expenses. Also, if the main revenue stream is a process output stream (i.e., a product stream), then this stream is also used to account for a product failure rate (see below).

The revenue streams, the main revenue stream, and the calculation options for their unit selling price or processing fee, can be specified through the Stream Classification Dialog; for more details, see 4.10 Classification of Input and Output Streams. Note that if the selling price or processing fee of a revenue stream is not set by user, the user can specify the selling price of registered pure components through the Pure Component Properties Dialog: Economics Tab; for more details on pure components, see 3.1 Pure Components.

The revenues associated with a revenue stream are calculated by multiplying the stream's selling price or processing fee by its revenue rate (i.e., its mass flow rate). The latter is either calculated by the program as part of the simulation or set by user (if it is a process input stream, or the flow demand for that stream is specified by one or more operations that use it). Particularly, if a process output stream is specified as the main revenue stream, the revenue rate of that stream is decreased by a fraction corresponding to the product failure rate. The product failure rate can be specified through the Economic Evaluation Parameters Dialog: Production Level Tab; for more details, see 9.3l Failed Product Disposal Cost.

GENERATED POWER DENOTED AS REVENUE

Power generation procedures are the only process steps that can contribute to revenues through the sale of electricity; for more details, see 9.4c Power Generation Procedures.

The revenues associated with the sale of generated power denoted as revenue are calculated by multiplying the fraction of total generated power in the process that is not recycled by its unit selling price:

$$\text{Revenues} = (1 - \%\text{Recycled}) \times \text{Power} \times \text{Selling Price} \qquad \text{eq. (9.18)}$$

The percentage of recycled power indicates the amount of electricity that is not sold to a grid but is used instead in the process to partially compensate for its power requirements. Thereby, it reduces the operating expenses of the process. The savings associated with recycling of generated power are calculated as:

$$\text{Savings} = \%\text{Recycled} \times \text{Power} \times \text{Purchasing Price} \qquad \text{eq. (9.19)}$$

The total annual savings that result from recycling of generated power are used to calculate the net annual operating cost of a process; for more details, see 9.3p Net Annual Operating Cost.

ANNUAL REVENUES

The annual revenues of a project are calculated as the sum of the revenues of all streams and generated power types that are denoted as revenue. In addition, a *unit production (or processing) revenue* can be calculated by dividing the total annual revenues by the selected flow basis (total flow or component flow) of the stream that is specified as the 'Unit Reference' stream through the Rate Reference Flows Dialog: Unit Reference tab. To display this dialog, select menu **Tasks \ Rate Reference Flow(s)**. Depending on whether the selected stream is a process input or output stream, the corresponding unit revenue is denoted as 'processing' or 'production', respectively; for more details, see 'Main Product/Revenue Rate Stream' on page 4-29.

Here is where you can find relevant figures:

- The total annual revenues and the unit production (or processing) revenue are shown in the Executive Summary Dialog: Summary Tab, the Executive Summary Dialog: Revenues / Credits / Savings Tab, and Sections 1 (Executive Summary) and 10 (Profitability Analysis) of the Economic Evaluation Report (EER).

- The annual revenue rates, unit selling prices and annual revenues of individual streams and generated power types denoted as revenue are listed in the Executive Summary Dialog: Revenues / Credits / Savings Tab and in Section 10 (Profitability Analysis) of the Economic Evaluation Report (EER).

Note that Section 10 (Profitability Analysis) of the Economic Evaluation Report (EER) is only available if the revenues of a project are positive.

9.4b Credits

These include proceeds from plant operation that are subtracted from the operating cost instead of adding them to the plant's revenues. Credits may include proceeds from:

- the sale of main and side products,
- the sale of generated electricity.
- the sale of heat as a heat transfer agent.

CREDIT STREAMS

In SuperPro Designer, the first credit source is determined based on the flow and unit price of streams that are specified as being 'credit' streams. The credits associated with a credit stream are calculated by multiplying the stream's selling price by its mass flow rate. The latter is either calculated by the program as part of the simulation or set by user (if it is a process input stream or if the flow demand for that stream is specified by one or more operations that use it). The classification of streams as credit streams and the calculation options for their unit selling price can be specified through the Stream Classification Dialog; for more details, see 4.10 Classification of Input and Output Streams. Note that if the selling price of a credit stream is not set by user, the user can specify the selling price of registered pure components through the Pure Component Properties Dialog: Economics Tab; for more details on pure components, see 3.1 Pure Components.

GENERATED POWER DENOTED AS CREDIT

The second credit source is determined based on the amount and unit price of generated power that is denoted as 'credit'. Power generation procedures are the only process steps that can contribute to credits through the sale of electricity; for more details, see 9.4c Power Generation Procedures.

The credits associated with the sale of generated power denoted as credit are calculated by multiplying the fraction of total generated power in the process that is not recycled by its unit selling price:

$$\text{Credits} = (1 - \%\text{Recycled}) \times \text{Power} \times \text{Selling Price} \qquad \text{eq. (9.20)}$$

The percentage of recycled power indicates the amount of electricity that is not sold to a grid but is used instead in the process to partially compensate for its power requirements. Thereby, it

reduces the operating expenses of the process. The savings associated with recycling of generated power are given by eq. (9.19):

$$\text{Savings} = \%\text{Recycled} \times \text{Power} \times \text{Purchasing Price} \qquad \text{eq. (9.19)}$$

The total annual savings that result from recycling of generated power are used to calculate the net annual operating cost of a process; for more details, see 9.3p Net Annual Operating Cost.

HEAT TRANSFER AGENT CREDITS

Heat transfer agent credits can be created by recovering the heat from a very hot operation in the process. When this heat is matched with a heating agent, under certain temperature conditions, and if the heat exceeds the total demand in this heating agent, then the agent can be credited by the excess duty load times the unit cost of the heating agent (based on an energy basis). For more details, see 9.6 Energy Recovery.

ANNUAL CREDITS

The annual credits of a project are calculated as the sum of the credits of all streams recovered heat and generated power types that are denoted as credit.

Here is where you can find relevant figures:

- The total annual credits are shown (if these are non-zero) in the Executive Summary Dialog: Summary Tab, the Executive Summary Dialog: Revenues / Credits / Savings Tab, and Sections 1 (Executive Summary) and 10 (Profitability Analysis) of the Economic Evaluation Report (EER).
- The annual credit rates, unit selling prices and annual credits of individual streams and generated power types denoted as credit are listed in the Executive Summary Dialog: Revenues / Credits / Savings Tab and in Section 10 (Profitability Analysis) of the Economic Evaluation Report (EER).

Note that Section 10 (Profitability Analysis) of the Economic Evaluation Report (EER) is only available if the revenues of a project are positive.

9.4c Power Generation Procedures

Power generation procedures are the only process steps that can contribute to revenues through the sale of electricity. These include:

- Power Generation in a Single-Stage Steam Turbine
- Power Generation in a Multi-Stage Steam Turbine
- Power Generation in a Single-Stage Gas Turbine
- Power Generation in a Multi-Stage Gas Turbine

For each unit procedure, the user specifies the generated power type in the corresponding operation. The amount of generated power is either calculated by the program as part of the simulation (in design mode of equipment) or specified by the user (in rating mode of equipment). For each generated power type included in the process, the user also specifies:

- its unit purchasing price,

- its unit selling price,
- whether it should be treated as revenue or credit,
- whether a percentage of generated power is recycled, and
- the percentage of power that is recycled.

For generated power types that are currently used in a process, the above properties can be viewed or edited through the List of Power Types Currently Generated by the Process dialog. To display the 'Power Resources Currently Generated' dialog, do one of the following:

- click **Process Options ▸ Resources ▸ Power Types Generated** on the **Edit** menu, or
- right-click on the flowsheet to bring up its context menu and click **Resources ▸ Power Types Generated**.

To edit the properties of a power type, double-click on the corresponding item on the list; for more details, see 6.9 Power.

Note that new power types can be created and added to power types databank of the 'User' database. To access the 'Power Types Databank' dialog, click **Power Types** on the **Databanks** menu. To edit the properties of a user-defined power type, switch to the 'User' database and double-click the desired item on the list; for more details, see 15.8 Power Types Databank.

You may choose to use site power types in a process section. You can store power types with distinct properties behind model database sites and allocate the site with the most appropriate power types to the relevant section(s) within your recipe; for more details, see 15.13 Sites & Resources Databank.

9.4d Savings

Savings to the annual operating cost can be calculated in the process. These funds can orginate from:

- Recycled power
- Recovered energy

RECYCLED POWER

If power is generated in the process the user may choose to recycle it, thus reducing the operating costs due to power demands. For more details see also Generated Power Denoted as Revenue and Generated Power Denoted as Credit.

RECOVERED ENERGY

Energy in the form of heat can be recovered from operations requiring cooling and matched with operations requiring heat or actual heating agents. This will create savings from the source and the recipient side. For more details see also Energy Recovery.

9.5 PROFITS

A profitability analysis is performed to determine the annual net profits of an investment. A cash flow analysis is performed to determine the net profits and net cash flow for each year over the lifetime of a project. These are described in detail below:

9.5a Profitability Analysis

The profitability analysis calculations consist of determining the annual gross profit and the annual net profit of an investment, as well as key economic indicators, such as the gross margin, the return on investment (ROI), and the payback time.

Here is where you can find these figures:

- All figures are listed in Section 10 (Profitability Analysis) of the Economic Evaluation Report (EER). Note that this is only available if the revenues of a project are positive.
- The gross margin, ROI and payback time are also listed in Section 1 (Executive Summary) of the Economic Evaluation Report (EER) and in the Executive Summary Dialog: Summary Tab.

The calculation of these economic parameters is described below.

GROSS PROFIT

The annual gross profit of a project is calculated by subtracting the annual operating cost (AOC) from the total annual revenues:

$$\text{Gross Profit} = \text{Revenues} - \text{AOC} \qquad \text{eq. (9.21)}$$

For more details on the annual operating cost, see 9.3 Operating Cost; for more details on the annual revenues, see 9.4a Revenues.

INCOME TAXES

The annual income taxes are calculated as a percentage of the annual gross profit. The tax coefficient can be specified through the Economic Evaluation Parameters Dialog: Misc. Tab. The default income tax is 40%.

NET PROFIT

By default, the annual net profit of a project is calculated as the annual gross profit minus the annual income taxes plus the annual depreciation:

$$\text{Net Profit} = \text{Gross Profit} - \text{Taxes} + \text{Depreciation} \qquad \text{eq. (9.22)}$$

The annual depreciation is calculated based on the straight-line method; for more details, see 9.3o Depreciation. Note that if you would rather see in the net profit figure only “real” revenues and not the depreciation, which may be considered an artificial (or accounting) income, then

you can select the option to subtract depreciation from the net profit. This can be specified through the Economic Evaluation Parameters Dialog: Financing Tab.

GROSS MARGIN

The gross margin is a measure of profit that directly tells you what percentage of the annual revenues is gross profit. It is calculated by dividing the annual gross profit by the annual revenues:

$$\text{Gross Margin} = \frac{\text{Gross Profit}}{\text{Revenues}} \times 100 \qquad \text{eq. (9.23)}$$

For more details on the annual revenues, see 9.4a Revenues.

RETURN ON INVESTMENT

The return on investment (ROI) is another profitability measure used to evaluate the viability of an investment or to compare the profitability of a number of different investments. It is calculated by dividing the annual net profit by the total capital investment charged to this project:

$$\text{Return on Investment (ROI)} = \frac{\text{Net Profit}}{\text{Total Investment}} \times 100 \qquad \text{eq. (9.24)}$$

If an investment does not have a positive ROI, or if there are other opportunities with a higher ROI, then the investment should not be undertaken.

For more details on the total capital investment charged to this project, see 9.2f Capital Investment Charged to This Project.

PAYBACK TIME

The payback time is a measure of the time needed for the total capital investment to be exactly balanced by the cumulative net profits. It is calculated by dividing the total capital investment charged to this project by the annual net profit:

$$\text{Payback Time (in years)} = \frac{\text{Total Investment}}{\text{Net Profit}} \qquad \text{eq. (9.25)}$$

The shorter the payback time, the more attractive the project appears to be.

For more details on the total capital investment charged to this project, see 9.2f Capital Investment Charged to This Project.

9.5b Cash Flow Analysis

The cash flow analysis calculations consist of determining the annual net cash flow over the lifetime of a project. The results of the analysis are presented in the Cash Flow Analysis Report (CFR). The calculations involved in the cash flow analysis are described below.

NET CASH FLOW

For each year before the start of operation (i.e., during construction and startup), the net cash flow will consist of the amount of money borrowed (debt financing) minus capital expenses for that year:

$$NCF = NCF_{con} = \text{Debt Financing} - \text{Capital Expenses} \qquad \text{eq. (9.26)}$$

For each operating year during the expected lifetime of the project, the net cash flow will also include the net profit and, optionally, depreciation:

$$NCF = NCF_{con} + \text{Net Profit} + \text{Depreciation} \qquad \text{eq. (9.27)}$$

Note that the last term will only be included if depreciation is subtracted from the net profit; for more details, see 9.5a Profitability Analysis.

The starting year of construction, the construction period, the startup period and the project lifetime can be specified through the Economic Evaluation Parameters Dialog: Time Valuation Tab. The default starting year of construction is the present year. The default construction period, startup period and project lifetime are 30 months, 4 months and 15 years, respectively.

CAPITAL EXPENSES

For each year during the expected lifetime of the project, the capital expenses may generally include the fractions of DFC-related expenses, up-front R&D (UFRD), up-front royalties (UFR), startup & validation cost (SC) and working capital (WC) that contribute to that year's capital expenses according to a predefined time schedule.

$$\text{Capital Expenses} = f_c \times \left[\left(1 - f_s\right) \times f_p \times \text{DFC} \right] + \text{UFRD} + \text{UFR} + \text{SC} + \text{WC} \qquad \text{eq. (9.28)}$$

where:

- f_p is the fraction of the process's DFC that is assigned to this project,
- f_s is the salvage fraction of the project's DFC, and
- f_c is the fraction of the project's DFC that is added to the year's capital expenses.

In SuperPro Designer, the fractions f_c can be specified for a maximum period of five years from the start of the project. The total UFRD is included in the capital expenses of the first year of the project. The total UFR, SC and WC are included in the capital expenses of the first year of operation. The salvage fraction of the project's DFC is only subtracted from the project's DFC in the last year of the project. In that year, the working capital is also subtracted.

The fraction, f_p, of the process's DFC that is assigned to this project is calculated based on the corresponding fractions of section-level DFCs that are assigned to this project. These are specified either directly or on a unit-by-unit basis through the Capital Investment Dialog: Cost Alloc Tab; for more details, see 9.2f Capital Investment Charged to This Project. The salvage

fraction, f_s, of the project's DFC and the DFC outlay (fractions f_c) for the first five years of the project can be specified through the Economic Evaluation Parameters Dialog: Financing Tab.

The time schedule used to describe the DFC outlay can span up to five years.

The positive capital expenditure in the final year of the project is due to the salvage value of equipment and the return of the working capital.

The breakdown of capital outlay into individual capital expenses related to DFC, WC, UFRD and UFR for each year during the lifetime of a project are listed in Section 3 (Capital Outlay) of the Cash Flow Analysis Report (CFR).

DEBT FINANCING

For each year up to the first year of operation or up to fifth year of the project (if the start of operation is in more than five years), the debt financing term will include the fraction, f_d, of DFC-related capital expenses that comes from a loan and is in debt:

$$\text{Debt Financing} = DF_{DFC} = f_d \times \left(f_c \times f_p \times DFC\right) \qquad \text{eq. (9.29)}$$

For the first year of operation, the debt financing term will also include the corresponding fractions, f_w, f_{rd} and f_r of working capital (WC), up-front R&D (UFRD) and up-front royalties (UFR), respectively, that come from a loan and are in debt:

$$\text{Debt Financing} = DF_{DFC} + f_w \times WC + f_{rd} \times UFRD + f_r \times UFR \qquad \text{eq. (9.30)}$$

Note that these fractions are constant for each year. In other words, it is assumed that the fraction of capital expenses that comes from a loan (or, equivalently, the fraction of capital expenses that comes from equity financing) each year is the same. The fractions of the above capital cost elements that are in debt can be specified through the Economic Evaluation Parameters Dialog: Financing Tab.

The total amount, the percent that comes from equity financing, the percent that is in debt, the loan interest and the loan period for each of the DFC, WC, UFRD and UFR are listed in Section 2 (Loan Information) of the Cash Flow Analysis Report (CFR).

DEPRECIATION

SuperPro Designer depreciates the fraction of a section's DFC that is assigned to this project and has not been depreciated already minus its salvage value at the end of the project lifetime. The user also has the option to depreciate the section's startup and validation cost. The total depreciable amount for the entire project is calculated by summing-up the total depreciable amounts over all sections. This amount is spread over the depreciation period (starting from the first year of operation) based on a specified depreciation method. Available methods are the

straight-line method, the declining balance method, and the sum-of-the-years-digit method; for more details, see 9.3o Depreciation.

NET PROFIT

For each operating year during the expected lifetime of the project, the net profit will include the taxable income minus the income taxes plus the depreciation:

$$\text{Net Profit} = \text{Taxable Income} - \text{Taxes} + \text{Depreciation} \qquad \text{eq. (9.31)}$$

Note that if you would rather see in the net profit figure only "real" revenues and not the depreciation, which may be considered an artificial (or accounting) income, then you can select the option to subtract depreciation from the net profit. This can be specified through the Economic Evaluation Parameters Dialog: Financing Tab.

TAXABLE INCOME

For each operating year during the expected lifetime of the project, the taxable income will include the gross profit minus the total loan payments:

$$\text{Taxable Income} = \text{Gross Profit} - \text{Loan Payments} \qquad \text{eq. (9.32)}$$

GROSS PROFIT

For each operating year during the expected lifetime of the project, the gross profit will include the total revenues minus the total operating cost:

$$\text{Gross Profit} = \text{Revenues} - \text{Operating Cost} \qquad \text{eq. (9.33)}$$

REVENUES

For each operating year during the expected lifetime of the project, the revenues are calculated by multiplying the calculated annual revenues with the fraction, f_Q, of total capacity that corresponds to the operating capacity for that year, and with the months, t, of operation for that year (if it is the first year of operation):

$$\text{Revenues} = f_Q \times (t/12) \times \text{Annual Revenues} \qquad \text{eq. (9.34)}$$

The operating capacity profile during the project's operational period can be specified through theEconomic Evaluation Parameters Dialog: Production Level Tab. The default value is 100% for all years. The actual months of operation during the first year of operation are calculated by subtracting any remaining months to complete construction and startup from the twelve months of the year. For a description of the calculation of annual revenues, see 9.4a Revenues.

OPERATING COST

For each operating year during the expected lifetime of the project, the operating cost is calculated by multiplying the calculated annual variable operating cost, AOC_V, with the fraction, f_Q, of operating capacity for that year and with the months, t, of operation for that year (if it is the first year of operation) and adding the annual fixed operating cost, AOC_F to the product:

$$\text{Operating Cost} = f_Q \times (t/12) \times AOC_V + AOC_F \qquad \text{eq. (9.35)}$$

For a definition of variables f_Q and t, see 'Revenues' on page 9-39. The annual variable operating cost is calculated as the annual operating cost minus the labor-dependent cost and the facility-dependent cost. The annual fixed operating cost is calculated as the labor-dependent cost plus the facility-dependent cost minus the annual depreciation. The latter term is subtracted because a different depreciation method than the straight-line method may be employed in cash flow analysis calculations. For more details on the calculation of the above cost elements, see 9.3 Operating Cost.

INCOME TAXES

For each operating year during the expected lifetime of the project, the income taxes are calculated as a percentage of the taxable income. The tax coefficient can be specified through the Economic Evaluation Parameters Dialog: Misc. Tab.The default income tax is 40%.

No tax is assessed for years where the cumulative net profit is negative.

LOAN PAYMENTS

The total annual loan payments will include the annual payments of the individual debts owed for the fractions of DFC-related expenses, working capital (WC), up-front R&D (UFRD) and up-front royalties (UFR) that come from a loan. The annual payment of each debt is calculated for each operating year during the loan period of each debt as:

$$\text{Annual Loan Payment} = \text{Total Debt} \times \frac{i}{1-(1+i)^{-t}} \qquad \text{eq. (9.36)}$$

where:

- i is the loan interest, and
- t is the loan period in years.

The total debts owed for WC, UFRD and UFR correspond to the respective specified fractions of these capital cost elements that come from a loan (see 'Debt Financing' on page 9-38 for more details). However, the total debt owed for DFC-related expenses must account for the accrued interest of the amount borrowed during construction (according to the specified DFC layout and the specified fraction of DFC-related expenses that comes from a loan) since the payment of this amount will only start after the first year of operation. For each year, *k*, of the

project up to the fifth year (or, up to the expected lifetime of the project if this is less than five years), the debt owed for DFC-related expenses is calculated as:

$$\text{Debt}_{\text{DFC},k} = \text{DF}_{\text{DFC}} \times (1 + i)^{t_c - k} \qquad \text{eq. (9.37)}$$

where:

- DF_{DFC} is the debt financing term for DFC-related expenses (see 'Debt Financing' on page 9-38 for more details), and
- t_c is the full years of construction (i.e., the years of accrued interest).

The total debt owed for DFC-related expenses is calculated as the sum of the corresponding debts over all years considered.

The loan fraction, loan period and loan interest for each capital cost element considered can be specified through the Economic Evaluation Parameters Dialog: Financing Tab.

The full years of construction are calculated based on starting year of construction, the construction period, the startup period and the project lifetime can be specified through the Economic Evaluation Parameters Dialog: Time Valuation Tab.The default starting year of construction is the present year. The default construction period, startup period and project lifetime are 30 months, 4 months and 15 years, respectively.

The breakdown of loan payment into individual loan payments of the debts owed for the DFC, WC, UFRD and UFR for each year during the lifetime of a project are listed in Section 4 (Breakdown of Loan Payment) of the Cash Flow Analysis Report (CFR).

NET PRESENT VALUE

The net present value (NPV) is a profitability measure used to evaluate the viability of an investment or to compare the profitability of a number of different investments. It represents the total value of future net cash flows during the life time of a project, discounted to reflect the time value of money at the beginning of a project (i.e., at time zero). It is calculated for three different interest rates (low, medium and high) using the following formula:

$$\text{NPV} = \sum_{k=1}^{N} \frac{\text{NCF}_k}{(1 + i)^k} \qquad \text{eq. (9.38)}$$

where:

- i is the interest rate,
- NCF_k is the net cash flow in year k, and
- N is the project lifetime (in number of years).

If an investment does not have a positive NPV, or if there are other opportunities with a higher NPV, then the investment should not be undertaken.

The three interest rates can be specified through the Economic Evaluation Parameters Dialog: Time Valuation Tab. The default values for the low, medium and high interest rates are 7%, 9% and 11%, respectively. The specified interest rates and the calculated NPV for each rate are listed in Section 1 (Cash Flow Analysis) of the Cash Flow Analysis Report (CFR). In addition, the NPV at the low interest rate is shown in the Executive Summary Dialog: Summary Tab.

INTERNAL RATE OF RETURN

The internal rate of return (IRR), which is also known as discounted cash rate of return (DCRR) is calculated based on cash flows before and after income taxes. The cash flow after income taxes corresponds to the net cash flow. The cash flow before income taxes is calculated as the net cash flow plus the income taxes. The method is analogous to the NPV method, but instead of asking what the NPV is for a prescribed interest rate, we seek a value of the interest rate which will make the NPV of all the cash flows just equal to zero. The values of IRR before and after taxes are listed in Section 1 (Cash Flow Analysis) of the Cash Flow Analysis Report (CFR). The IRR after taxes is also shown in the Executive Summary Dialog: Summary Tab.

9.6 ENERGY RECOVERY

From version 9.0 of SuperPro the user has the option to recover energy in the form of heat. This heat can be exchanged between operations that require cooling and operations that require heat in order to improve the efficiency and economics in the process. Conserving energy will significantly reduce overall utility usage and associated utility costs. Energy recovery can be accomplished in two ways:

(a) by matching heat source locations requiring cooling with on or more locations needing heat, or

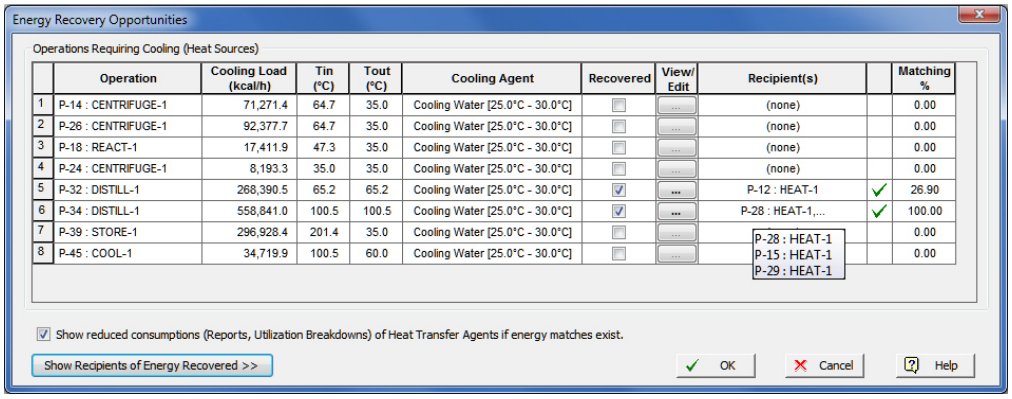
(b) by matching heat source locations requiring cooling with actual heating agents

Exchanging of heat can be performed directly by using a heat exchanging unit procedure and connecting the relevant input and output streams, and defining operational data for the procedure. However if there are many possible heat exchanging opportunities in the process the energy recovery method allows you to more quickly and easily define the heat recovery network. In addition, there are fewer “extraneous” stream lines and unit procedure icons on the flowsheet, and the whole heat recovery network can be easily viewed and modified from a single interface dialog.

The energy recovery matching can be done through the Energy Recovery Opportunities Dialog. To display this dialog, do one of the following:

- click **Process Options ▸ Resources ▸ Energy Recovery...** on the **Edit** menu, or
- right-click on the flowsheet to bring up its context menu and click **Resources ▸ Energy Recovery...**.

On the interface that appears (see Figure 9.2) the user may see a list of all the operations requiring cooling in the process. These locations are the potential heat sources which can be matched with suitable cold operations requiring heat or suitable heating agents.


Energy Recovery Opportunities
Operations Requiring Cooling (Heat Sources)
Show reduced consumptions (Reports, Utilization Breakdowns) of Heat Transfer Agents if energy matches exist.
Show Recipients of Energy Recovered >>
OK
Cancel
Help

	Operation	Cooling Load (kcal/h)	Tin (°C)	Tout (°C)	Cooling Agent	Recovered	View/ Edit	Recipient(s)		Matching %
1	P-14 : CENTRIFUGE-1	71,271.4	64.7	35.0	Cooling Water [25.0°C - 30.0°C]	☐	...	(none)		0.00
2	P-26 : CENTRIFUGE-1	92,377.7	64.7	35.0	Cooling Water [25.0°C - 30.0°C]	☐	...	(none)		0.00
3	P-18 : REACT-1	17,411.9	47.3	35.0	Cooling Water [25.0°C - 30.0°C]	☐	...	(none)		0.00
4	P-24 : CENTRIFUGE-1	8,193.3	35.0	35.0	Cooling Water [25.0°C - 30.0°C]	☐	...	(none)		0.00
5	P-32 : DISTILL-1	268,390.5	65.2	65.2	Cooling Water [25.0°C - 30.0°C]	☑	...	P-12 : HEAT-1	✓	26.90
6	P-34 : DISTILL-1	558,841.0	100.5	100.5	Cooling Water [25.0°C - 30.0°C]	☑	...	P-28 : HEAT-1,...	✓	100.00
7	P-39 : STORE-1	296,928.4	201.4	35.0	Cooling Water [25.0°C - 30.0°C]	☐	...			0.00
8	P-45 : COOL-1	34,719.9	100.5	60.0	Cooling Water [25.0°C - 30.0°C]	☐	...			0.00

P-28 : HEAT-1
P-15 : HEAT-1
P-29 : HEAT-1

Figure 9.2: Energy Recovery Opportunities Dialog

ECONOMIC FIGURES AFFECTED BY HEAT RECOVERY

Linking heat source operations with cold operations requiring heat or heating agents, will have an impact on the economics. By default the consumptions of heat transfer agents in the process as well as in the reports, charts and utilization breakdown trees, are not affected by any heat recovery matches. Not unless the user explicitly specifies it by checking the option **Show reduced consumptions (Reports, Utilization Breakdowns) of Heat Transfer Agents if energy matches exist.** on the Energy Recovery Opportunities Dialog or the option **Show reduced consumption of agents due to heat recovery.** on the Utility Selection For Consumption Chart dialog. In this case the heat matches will have an impact on the net total annual operating cost in the form of savings (see 9.3p Net Annual Operating Cost). Any savings existing in the process can be seen on the Executive Summary Dialog and in the Profitability Analysis section of the 12.4a Economic Evaluation Report (EER).

If heat source operations are matched with heat transfer agents and the heat source can provide more heat than the demand of the heating agent then the excess heat can be used as credit. A credit price can be given to the heating agent through the properties of the heat transfer agent. The credit produced can also affect the net annual operating cost of the process.

When however the user chooses to show the consumptions of heat transfer agent utilities reduced by any heat recovery matches, then the economics will be directly affected. This means any economic figures that take in account the cost of heat transfer agents and are reported in SuperPro will be reduced.

9.7 REPORTING OF ECONOMIC FIGURES

The key results of the economic calculations are shown in the Executive Summary Dialog. To access this dialog, click **Executive Summary** on the **View** menu.

In addition, the following economic reports can be generated:

- Economic Evaluation Report (EER)
- Cash Flow Analysis Report (CFR)
- Itemized Cost Report (ICR)

The Economic Evaluation Report (EER) includes an executive summary that contains the key results of economic analysis for a project, detailed breakdowns of annual capital and operating costs, and the main input and output data of profitability analysis. To generate this report, click **Economic Evaluation (EER)** on the **Reports** menu; for more details on the contents of this report, see12.4a Economic Evaluation Report (EER).

The Cash Flow Analysis Report (CFR) includes loan information and breakdowns of capital outlay, loan payment and cash flow for each year over the expected lifetime of a project. To generate this report, click **Cash Flow Analysis (CFR)** on the **Reports** menu; for more details on the contents of this report, see 12.4b Cash Flow Analysis Report (CFR).

The Itemized Cost Report (ICR) contains various cost breakdowns of the fraction of the total annual operating cost (AOC) that consists of the cost items that are calculated at the process section level. To generate this report, click **Itemized Cost (ICR)** on the **Reports** menu; for more details on the contents of this report, see 12.4c Itemized Cost Report (ICR).

9.8 CURRENCY

The default currency used in a new process simulation or the 'User' database for viewing or editing cost-related information is the 'US Dollar'. This is the only currency type that is available in the Currencies Databank of the system ('Designer') database.

You may create new currency types with specific properties (name, symbol and exchange rate to US$) and add them to the Currencies Databank. This can be done through the 'Currencies Databank' dialog. To access this dialog, click **Currencies** on the **Databanks** menu. Through the same dialog, you may specify the default currency for the 'User' database; for more details, see 15.12 Currencies Databank.

In order to use a new currency in a process simulation, you must select it through the Currency Selection Dialog. To access this dialog, do one of the following:

- click **Process Options ▸ Currency** on the **Edit** menu, or
- right-click on the flowsheet to bring up its context menu and click **Currency**.

From that moment onward, all prices or cost-related items are going to be accepted in that currency. Also, results (operating cost, capital cost, etc.) in charts as well as reports will be presented in the selected currency.

9.9 REFERENCES

1. Valle-Riestra, J. F. Project Evaluation in the Chemical Process Industries. McGraw-Hill, NY, 1983.
2. Peters, Max S., and Klaus D. Timmerhaus Plant Design and Economics for Chemical Engineers. 4th edition, McGraw-Hill, NY, 1991.

and match it with multiple heat recipient operations if feasible from the listTo match a heat recipient operation with a heat source you must double click on the check-box cell at the beginning of each row. Once checked the last column (Match '%') will be updated showing the percentage of load that has been saved. At the same time the Available for Transfer heat will have changed, leaving less load to be matched with another operation. Continuing to match heat recipient operations with the same heat will eventually deplete all the heat, which will cause the rest of the rows to be disabled and be greyed out. In order to match the heat with one of the rows that has been disabled, the user must un-check one of the matched operations to make some heat load available again.

All of the heat from a hot operation can be matched with one Heat Transfer Agent, simply by clicking on the row of the utility.

10

EMISSIONS

Another important aspect of SuperPro Designer is that it performs venting and emission calculations in batch and continuous operations based on rigorous thermodynamic VLE models. Moreover, there are special (dedicated) mass-transfer and empirical models for calculating emissions in wastewater treatment operations and cooling towers. In a future release, SuperPro will offer the option to generate emission reports based on the EPA/MACT guidelines.

Emissions documentation provides information on the following topics:

- Vent/Emission Calculations In Batch and Continuous Operations
- Special Emission Models For Wastewater Treatment Processes and Cooling Towers
- Emission Calculations Based On EPA/MACT Guidelines
- Emissions Report (EMS)
- Emission Limits
- Emission Interfaces

10.1 VENT/EMISSION CALCULATIONS IN BATCH AND CONTINUOUS OPERATIONS

SuperPro Designer performs venting and volatile organic compound (VOC) emission calculations for several batch operations that are common in the pharmaceutical and specialty chemical industries. Furthermore, venting is available for several continuous operation including reactions, storage, etc. Operations that have the option to perform vent/emissions calculations are those that can cause a change in the vapor phase while executed in equipment that accumulates material. Typical examples are Charge, Transfer In and Pull In operations executed in the context of Batch Vessel Procedures that cause the displacement of freeboard gases. If venting occurs then emission calculations are also possible to account for VOC gases that are swept away by the freeboard gases.

Operations that can perform vent/emissions will include a 'Vent/Emissions' tab in their dialog like the one shown in Figure 10.1 for the Charge operation. Venting is optional and, by default, assumed to be off except for certain operations including Purging / Inerting, Evacuation, Batch Stoichiometric Fermentation with aeration etc., that absolutely require the removal of gases. A closed vent corresponds to a closed-valve operation that does not allow any gases to escape, making pressure built-up possible. Note that, when not explicitly set by the user, the operating pressure is calculated by SuperPro Designer based on the amount of freeboard gases and the available equipment headspace.

If venting is turned on, the user can select the port through which gases will escape. By default, this port is the equipment's 'vent/emissions' port (usually the top output port when available) but any other output port could be selected, provided that no other operation in the procedure uses it for purposes other than venting. Sharing of the same port among different operations for venting is possible. The streams connected to these vent/emission ports are by default classified as 'emission' streams (i.e., the 'Auto-Tag Stream' option is checked by default in the 'Vent/Emissions' tab of an operation).Vent streams are always assumed to be 100% vapor and their physical state options are locked (i.e., cannot be changed by the user).

The program allows for the selection of a venting policy namely:

- open vessel (atmospheric) operation or,
- pressurized vessel operation with a user-specified relief valve setting

In the case of the open vessel, the pressure inside the equipment during the corresponding operation is assumed to be equal to the ambient pressure even if an amount of air needs to introduced into the equipment to equalize the pressure. This is a common scenario in operations where the temperature of the equipment contents decreases (e.g., Batch Cooling) or material is removed (e.g., Transfer Out). In the pressurized vessel case, gases can only escape if the pressure exceeds the relief-valve setting but air cannot flow into the equipment. In other words, the pressure of the equipment contents can be lower or equal to the relief valve setting.

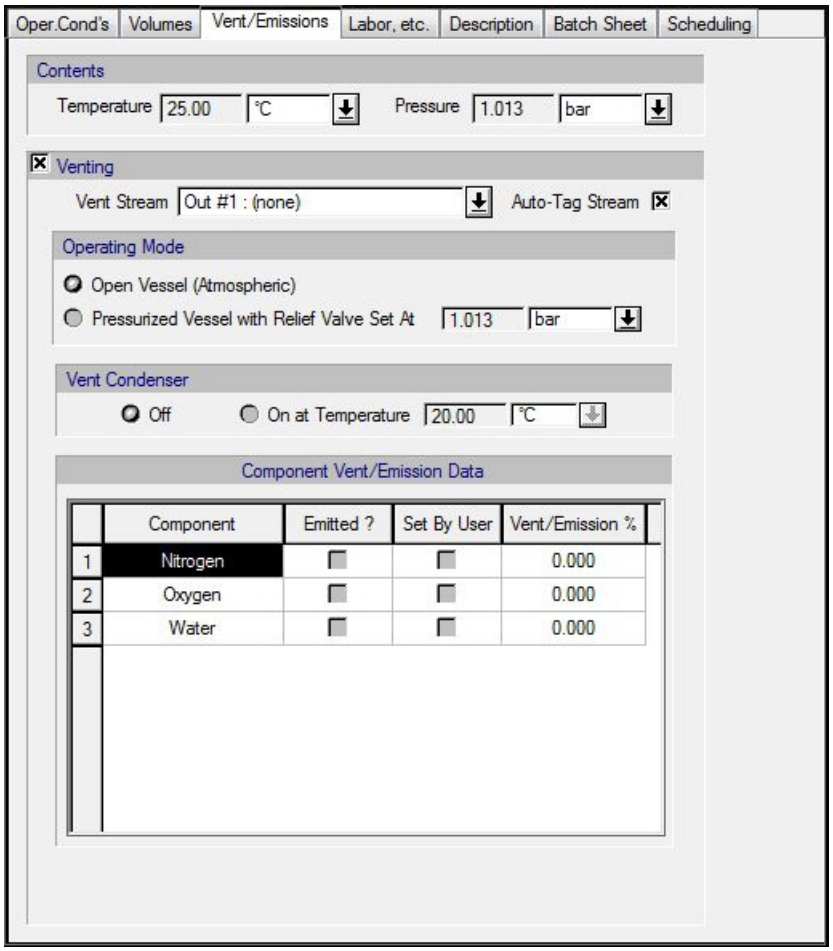


Figure 10.1: The 'Vent/Emissions' tab of the Charge operation.

SuperPro Designer offers the option for using a vent condenser with a user-specified temperature. By default, for new operations the vent condenser is off. To turn the vent condenser on, the user must check the respective radio button and specify an appropriate temperature. In general, the use of a vent condenser will result in a decreased concentration of VOCs in the vent stream.

Finally, the user must select which components are emitted and even specify the vented percentage for some of them. The Vent/Emission% expresses the portion of a component that is vented (e.g., from a vessel).

Components that are 100% in the vapor phase will be automatically checked by SuperPro as emitted. Specifying the Vent/Emission % for those components is not supported. The program will automatically un-check the Set By User checkbox and reset the respective value to 0.

It is important that components checked as Emitted possess some realistic VLE parameters (e.g., Antoine coefficients, critical properties etc.), otherwise emission calculations may fail. If such parameters cannot be provided, it is recommended that the Vent/Emission % of these components should be set by the user.

In the Vent/Emissions tab of reaction and fermentation operations there is also the option to sweep the contents with a sweep gas at a specified volumetric rate (see Figure 10.2).

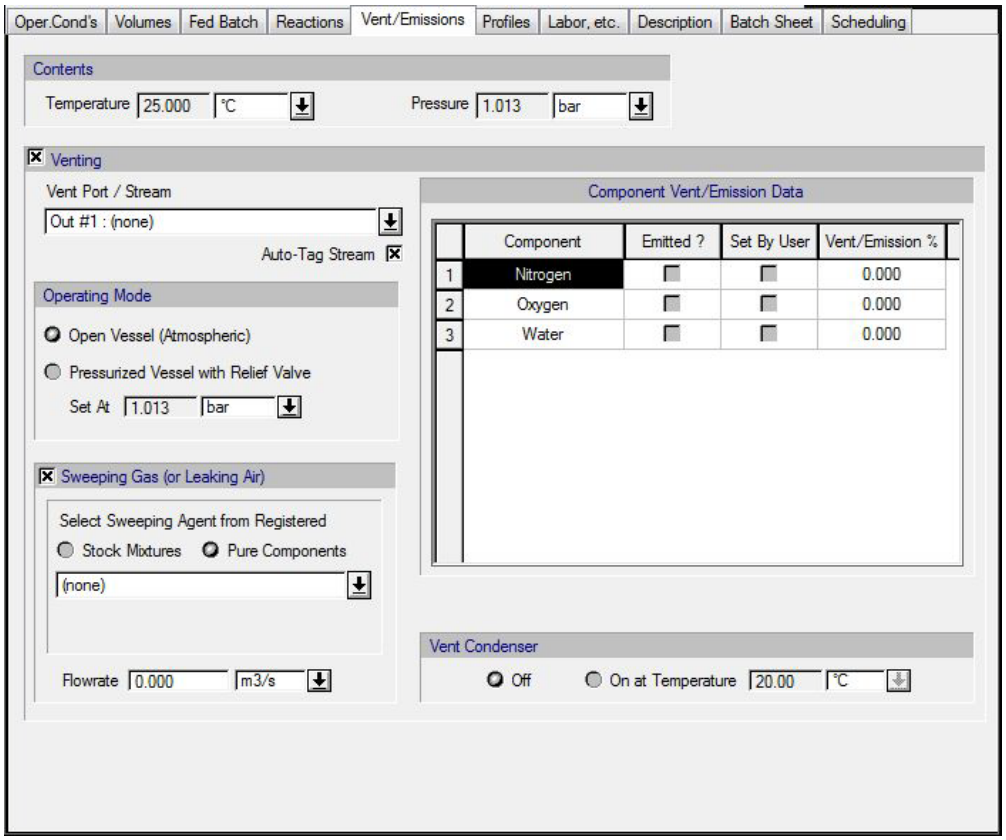


Figure 10.2: The 'Vent/Emissions' tab of the Batch Stoichiometric Fermentation operation.

If the Gas Sweep option is on, the entire amount of sweeping gas is mixed to the equipment contents before the Vent/Emission calculations are performed.

10.1a Calculation of Vent/Emissions Methodology in Batch Processes

The calculation of vent/emissions by SuperPro is based on the pressure conservation principle: *freeboard gases are removed from the equipment contents in order to satisfy the user-defined pressure setting*.

There is a substantial difference between SuperPro emission calculations and EPA emission calculations. SuperPro emission calculations are pressure-driven in the sense that the amount emitted is determined by the program in order to maintain pressure to the desired value. On the other hand, EPA emission calculations are volume-driven in the sense that the amount (volume) of emissions is pre-determined (e.g., by the amount of displaced gas or sweep gas). As a result, EPA emission calculations result in pressure inconsistencies.

Freeboard gases are removed according to the principles described below:

1. After the solution of the operation's mas and energy balances, the program determines the physical state of the equipment contents at their respective temperature and pressure *based on a Rigorous VLE model*. If the operation uses the Shortcut PS toolbox then the physical state is going to be determined by the Raoult's law model. Otherwise, the same VLE model used by the operation will be employed. This principle is called the *Raoult's law-or-better rule*. Subsequently, the composition of the vent stream is assumed to be equal to the composition of the gas phase inside the equipment.
2. For operations like Batch Heating, Evacuation or Venting where there is an implied gradual change in temperature or pressure, an average vent stream concentration is determined by advancing from the initial to the final condition in 5 homogeneous steps. Clearly, the average vent stream composition will be different from the composition of the gas phase of the vessel contents at the end of the operation.
3. If the vent condenser is on, then the vent stream is re-flashed at the corresponding temperature so that a new composition is acquired.
4. Given the composition of the vent stream, the program will calculate the amount that must be vented so pressure of the remaining gases inside the equipment headspace is matches the desired value. Notice that in the case described in point 2 above, this is not a straightforward calculation but requires an iterative procedure (e.g., a Newton-Raphson).

In general, when an operation uses the shortcut toolbox, the actual pressure of the equipment contents after venting will be slightly different than the displayed value because the physical state of the equipment contents as calculated by the shortcut toolbox will be different from the respective physical state as calculated by Raoult's Law.

10.1b Calculation of Vent/Emissions Methodology in Continuous Processes

In continuous operations where the vent is open, the entire amount of the gas phase (as inferred by the PS toolbox of the operation) will be directed to the vent stream. Otherwise, both the liquid and the gas portion of the contents will exit from the same stream. See Vent/Emission Calculations In Batch and Continuous Operations.

10.2 SPECIAL EMISSION MODELS FOR WASTEWATER TREATMENT PROCESSES AND COOLING TOWERS

SuperPro Designer is equipped with dedicated models for calculating VOC emissions from wastewater treatment plants and cooling. There are five types of emission calculation models in the current version of the software:

1. The first type includes emissions from tanks and basins with *quiescent surfaces* (e.g., equalizers, neutralizers, clarifiers, thickeners, flotation, and oil separation units). The removal of VOC vapor(s) from tanks with quiescent surfaces occurs due to natural volatilization, i.e., mass transfer across open surfaces.
2. The second type includes emissions from *aerated tanks* equipped with surface or diffused aeration systems. The removal of VOC vapor(s) from such tanks occurs due to surface volatilization for mechanically aerated systems or due to stripping for tanks with diffused aeration systems.
3. The third type includes emissions from *trickling filters*. Trickling filters are modeled as packed-media systems, in which volatilization is the primary removal mechanism for all VOC gases. Note that this is a conservative assumption for compounds that are biodegradable.
4. The fourth type includes emission calculation models for *junction boxes*. Junction boxes combine wastewater streams flowing into a treatment plant. These boxes are usually open to the atmosphere and VOC emissions occur in a similar manner as emissions from quiescent surface tanks.
5. Finally, the fifth type includes emission calculation models for *cooling towers*. The inlet water stream in cooling towers may contain volatile contaminants whose removal occurs in a similar manner as emissions from aerated tanks.

The emission models for trickling filters, junction boxes and cooling towers are described as part of their operation models; for more details, see:

- Trickling Filtration
- Junction Box Mixing
- Cooling in a Cooling Tower

A description of the VOC emission models for quiescent and agitated tanks follows below.

10.2a Quiescent Tanks - Emission Model

This model is available in the following operations:

- Clarification,
- Inclined Plate (IP) Clarification,
- Thickening,
- Flotation,
- Oil Separation, and
- Equalization.

VOC emissions from tanks with quiescent surfaces (clarifiers, thickeners, equalizers, etc.) occur due to natural volatilization, i.e., mass transfer across open surfaces. To account for VOC emissions in such tanks, you may either select the emission calculation model or simply specify the emission percent for a VOC component. The model calculates the rate of mass transfer across the air-wastewater interface as follows:

$$R_{vol} = K_L C_L A \qquad \text{eq. (10.1)}$$

where:

- R_{vol} is the rate of compound removal by volatilization (kg/s),
- K_L is the overall mass transfer coefficient (m/s),
- C_L is the VOC concentration in bulk liquid (kg/m^3), and
- A is the surface area of the tank (m2).

The value of C_L is calculated based on an overall component mass balance. The overall mass transfer coefficient depends upon the resistances of the gas and liquid phases. It is calculated as:

$$\frac{1}{K_L} = \frac{1}{k_l} + \frac{1}{H_C\, k_g} \qquad \text{eq. (10.2)}$$

where:

- k_l is the mass transfer coefficient of the liquid phase (m/s),
- k_g is the mass transfer coefficient of the gas phase (m/s), and
- H_c is the dimensionless Henry's law constant.

The value of H_c is retrieved from the pure components databank. Two different models have been implemented in order to calculate the mass transfer coefficients of the liquid phase. The first model, which is accepted by the US EPA, utilizes two correlations formulated by Springer et al. (1984). These are based upon the wind speed at ten meters (U_{10}) above the liquid surface and the fetch-to-depth ratio (F/D) of the tank under consideration. ‘Fetch’ is the linear distance across the impoundment (EPA, 1994).

For F/D < 51.2 (originally developed for 14 < F/D < 51.2),

$$k_l = \left(2.605\text{x}10^{-9}\ (F / D) + 1.277\text{x}10^{-7}\right) U_{10}^2 \left(\frac{D_w}{D_{ether}}\right)^{0.67} \qquad \text{eq. (10.3)}$$

And, for F/D > 51.2,

$$k_l = 2.611 \times 10^{-7} U_{10}^2 \left(\frac{D_{VOC}}{D_{ether}} \right)^{0.67} \quad \text{eq. (10.4)}$$

where:

- D_{VOC} is the diffusivity of the VOC component in water (m^2/s), and
- D_{ether} is the diffusivity of ether in water (m^2/s).

The above equations were validated by Springer et al. for $U_{10} > 3.25$ m/s and may lead to lower accuracy for $U_{10} < 3.25$ m/s.

The second model estimates k_l using the correlations developed by Mackay and Yeun (1983):

$$k_l = 1.0 \times 10^{-6} + 34.1 \times 10^{-4} \ (U^*) \ Sc_L^{-0.5} \qquad \text{for} \quad U^* > 0.3 \quad \text{eq. (10.5)}$$

$$k_l = 1.0 \times 10^{-6} + 144 \times 10^{-4} \ (U^*)^{2.2} \ Sc_L^{-0.5} \qquad \text{for} \quad U^* < 0.3 \quad \text{eq. (10.6)}$$

where:

$$U^* = (6.1 + 0.63 U_{10})^{0.5} \ U_{10} \quad \text{eq. (10.7)}$$

$$Sc_L = \frac{\mu_L}{\rho_L \ D_W} \quad \text{eq. (10.8)}$$

In both cases, the gas phase mass transfer coefficient is calculated using the equation developed by Mackay and Matasugu (Hwang, 1982):

$$k_g = 1.0 \times 10^{-3} + 46.2 \times 10^{-3} \ U^* \ Sc_G^{-0.67} \qquad \text{where} \quad Sc_G = \frac{\mu_G}{\rho_G \ D_a} \quad \text{eq. (10.9)}$$

where:

- μ_L is the viscosity of water (kg/m-s),
- μ_G is the viscosity of air (kg/m-s),
- ρ_L is the density of water (kg/cm^3),
- ρ_G is the density of air (kg/cm^3),

- D_w is the diffusivity of the VOC component in water (m^2/s), and
- D_a is the diffusivity of the VOC component in air (m^2/s).

The above properties are retrieved from the components databank.

References

1. U. S. Environmental Protection Agency (EPA). 1994. "Air Emissions Models for Waste and Wastewater" *Rep. EPA-453/R-94-080A.* Research Triangle Park, NC: Office of Air Quality Planning and Standards.
2. Springer, C., P. D. Lunney, and K. T. Valsaraj. 1984. "Emission of Hazardous Chemicals from Surface and Near Surface Impoundments to Air," Project Number 808161-02. Cincinnati, OH: U.S. Environmental Protection Agency (EPA), Solid and Hazardous Waste Research Division.
3. Mackay, D., and A. T. K. Yeun. 1983. "Mass Transfer Coefficient Correlations for Volatilization of Organic Solutes from Water," *Environmental Science and Technology.* 17: 211-217.
4. Hwang, S. T. 1982. "Toxic Emissions from Land Disposal Facilities," *Environmental Progress*. 1: 46-52.

10.2b Agitated Tanks - Emission Model

This model is available in the following operations:

- Pressure...,
- Well-Mixed (WM) Kinetic Aerobic Bio-Oxidation,
- Plug-Flow (PF) Stoichiometric Aerobic Bio-Oxidation, and
- Plug-Flow (PF) Kinetic Aerobic Bio-Oxidation.

In agitated tanks, such as aeration basins, VOC emissions result from surface volatilization and diffused air stripping (if diffused air is used for aeration). The general material balance equation for a component that biodegrades and is emitted is given by the following equation:

$$0 = (\text{Input}) - (\text{Output}) - \begin{pmatrix}\text{Biochemical}\\ \text{Oxidation}\end{pmatrix} - \begin{pmatrix}\text{Surface}\\ \text{Volatilization}\end{pmatrix} - \begin{pmatrix}\text{Diffused}\\ \text{Air}\\ \text{Stripping}\end{pmatrix} \qquad \text{eq. (10.10)}$$

Or

$$0 = QC_{in} - QC - Vr_b - K_L aVC - Q_a K_{eq} CF_{st} \qquad \text{eq. (10.11)}$$

where:

- Q is the liquid flow rate,
- V is the reactor volume,

- C_{in} is the inlet concentration,
- C is the outlet concentration (which is the same as the concentration in the reactor),
- r_b is the biodegradation rate,
- $K_L a$ is the overall mass transfer coefficient,
- Q_a is the air flow rate (in case of diffused aeration),
- K_{eq} is the equilibrium constant, and
- F_{st} is the saturation term (which represents the extent of saturation of the exiting gas stream).

In general, the biodegradation rate is a function of substrate concentration, oxygen concentration, and biomass concentration. Various expressions are available for the effect of substrate. The overall equation with a Monod-type substrate expression is written as follows:

$$r_b = K_{max}\left(\frac{C}{K_s + C}\right)\left(\frac{C_O}{K_O + C_O}\right)X \qquad \text{eq. (10.12)}$$

where:

- K_{max} is the maximum rate constant,
- K_s is the half saturation constant for the substrate,
- C_0 is the oxygen concentration,
- K_0 is the half saturation constant for oxygen, and
- X is the biomass concentration.

Alternative expressions for the substrate and oxygen terms are also available. The components databank includes data for K_{max} and K_s for a large number of chemical components; for more details, see 3.1e Pure Component Properties.

The overall mass transfer coefficient of a VOC component is estimated as a function of the oxygen mass transfer coefficient in wastewater, using a proportionality coefficient, ψ_M:

$$(K_L a)_{VOC} = \psi_M (K_L a)_{O2} \qquad \text{eq. (10.13)}$$

The value of $(K_L a)_{O2}$ in the wastewater is a user input to the program (parameter named 'Oxygen Mass Transfer Coefficient at 20 ^oC' on the Vent/Emissions tab).

The value of ψ_M is calculated by the following equation (Hsieh et al., 1993):

$$\psi_M = \psi\left(\frac{R_l}{R_t}\right) = \psi\left\{1 + \frac{1}{H_c \dfrac{k_g a}{k_l a}}\right\}^{-1} \qquad \text{eq. (10.14)}$$

where:

- ψ is a dimensionless proportionality constant,
- $k_l a$ is the mass transfer coefficient of the liquid phase (1/s), and
- $k_g a$ is the mass transfer coefficient of the gas phase (1/s).

The proportionality constant is calculated using the following equation (Corsi and Card, 1991):

$$\psi = \left(\frac{D_{voc}}{D_{O2}}\right)^n \qquad \text{eq. (10.15)}$$

where:

- D_{VOC} is the diffusion coefficient of a VOC component in water (m^2/s),
- D_{O2} is the diffusion coefficient of oxygen in water (m^2/s)., and
- n is an exponent.

The exponent n varies from 0.5 for penetration and surface renewal theories to 1.0 for the two-film theory (Corsi and Card, 1991). Typically, it has a value between 0.5 and 0.6 (Mihelcic et al., 1993). SuperPro Designer uses a default value of 0.6 for all emitted component. A different value can be specified for each component. The diffusion coefficients of components are retrieved from the components databank of the program; for more details, see 3.1e Pure Component Properties.

For mechanically aerated systems, the ($k_g a/k_l a$) ratio can be estimated using the following empirical equation (Hsieh et al., 1993):

$$\log_{10}\left(\frac{k_g a}{k_l a}\right) = -0.39664 \log_{10}(P/V) + 2.6776 \qquad \text{eq. (10.16)}$$

where:

- P is the mechanical power consumed for surface aeration, and
- V is the liquid volume of the aeration basin.

The ratio (P/V) is calculated by the program as part of the simulation. Alternatively, you have the option to set the value of the ($k_g a/k_l a$) ratio or set the value of the (R_l/R_t) ratio. This specification option and the exponent n are specified for each component through the 'Vent/Emissions' tab, and more specifically, through a component's 'Emission Model' dialog. To open this dialog, select a component by clicking on its row number and click the **Emission model** button which is available on this tab. By default, a (R_l/R_t) ratio equal to one is used for all emitted components.

For diffused aerated systems, the F_{st} term is calculated by the following equation:

$$F_{st} = 1 - \exp\left(\frac{\psi_M \left(K_L a\right)_{O_2} V}{H_c \, Q_g}\right) \qquad \text{eq. (10.17)}$$

To calculate ψ_M, you have the option to set either the value of the ($k_g a/k_l a$) ratio or the value of the (R_l/R_t) ratio. Again, these options are available through the 'Vent/Emissions' tab of the corresponding operation and they can be specified for each emitted component. The choice between surface air (mechanically aerated system) and diffused air (diffused aerated system) is specified through the 'Oper. Cond's' tab of the corresponding operation.

The equilibrium constant is estimated by:

$$K_{eq} = \frac{H}{RT} \qquad \text{eq. (10.18)}$$

where R is the universal gas constant and T is temperature.

The above equations are written for each chemical component entering an aeration basin. These constitute a set of non-linear equations, which is solved numerically to calculate the exit concentration and the emission rate of each component.

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10.3 EMISSION CALCULATIONS BASED ON EPA/MACT GUIDELINES

10.3a Displacement - Emission Model

This model accounts for emissions when a liquid mixture is transferred into a vessel. It is used to compute VOC emissions by the following operations:

- Charge,
- Transfer In,
- Pull In,
- Transfer Out,
- Pull Out,
- Charge (Solids),
- Transfer In (Solids),
- Pull In (Solids),
- Transfer Out (Solids), and
- Pull Out (Solids).

The model assumes that the displaced gas volume is equal to the volume of liquid transferred into the vessel. The receiving vessel may be empty or contain a liquid mixture from prior operations. The displaced gas is assumed to be saturated with VOC vapor(s) at the exit temperature. According to this model, the amount of a VOC component (i) emitted during one of the above operations is calculated using the following equation:

$$m_i = \frac{p_i (X_i)(MW_i)}{RT} V_r \qquad \text{eq. (10.19)}$$

where:

- m_i is the mass of the i-th component (in kg),
- p_i is the vapor pressure of the i-th component at temperature T (in Pa),
- X_i is mole fraction of the i-th component in the liquid mixture,
- MW_i is the molecular weight of the i-th component (in kg/kmol),
- V_r is the volume of displaced gas (in m^3),

- R is the ideal gas constant (8,314.5 J/kmol-K),
- T is the exit temperature (in K).

The vapor pressure, p_i, is calculated using Antoine's equation or DIPPR's polynomial expression depending on whether the component properties are retrieved from the SuperPro Designer or DIPPR databases, respectively; for more details, see D.1b Thermodynamic Properties of Pure Components and Chapter 15 (Databases & Databanks).

The exit temperature, T, is set equal to the temperature of the condenser. If no condenser is available, then, it is set equal to the final temperature of the liquid mixture (at the end of the addition). The temperature of the liquid mixture may change if the transferred liquid has a different temperature from that of the initial contents of the vessel.

Dividing m_i by the cycle time of the corresponding unit procedure yields the emission rate (in kg/h) of a component during an operation. If several operations of a unit procedure contribute to VOC emissions, the total emissions from that procedure are combined and averaged over its cycle time.

A component's emission rate during an operation is averaged over the cycle time of the corresponding procedure that contains the operation and not over the duration of the operation.

10.3b Evacuation - Emission Model

This model accounts for emissions when the pressure of a vessel is reduced. It is used to compute VOC emissions by the following operations:

- Evacuation,
- Purging / Inerting, and
- Batch Vaporization / Solvent Switch: Mat. Balance Tab (Solvent Switch Mode).

Note that the model assumes that there is no leakage of air into the vessel even if the final pressure is below atmospheric. It is also assumed that there is no temperature change during the operation and that the displaced gas is saturated with VOC vapor(s) at the exit temperature of the vessel. Essentially, it is assumed that during the operation the total number of VOC moles in the gas space does not change (the emitted moles are replaced by the newly vaporized ones) and that the pressure change is entirely due to removal of inert gases. According to this model, the moles of a VOC component (i) emitted during an 'Evacuate', 'Purge/Inert' or 'Vent' operation are calculated using the following equation:

$$n_i = \frac{p_i\,(X_i)}{P_{inert}} n_{inert} \qquad \text{eq. (10.20)}$$

where:

- n_i is the amount of the i-th component (in kmol),
- p_i is the vapor pressure of the i-th component at the exit temperature T (in Pa),
- X_i is the mole fraction of the i-th component in the liquid mixture,

- n_{inert} is the amount of inert gases removed during the operation (in kmol), and
- P_{inert} is the average partial pressure of inert gases during the operation (in Pa).

The partial pressure of inert gases is estimated by considering the initial and final pressure of the system as well as the vapor pressure of the volatile compounds (which does not change during the operation). The amount of inert gases removed is estimated using the following equation:

$$n_{inert} = V\Delta P/(RT) \qquad \text{eq. (10.21)}$$

where:

- V is the gas space volume,
- ΔP is the system pressure change, and
- T is the exit temperature.

Dividing n_i by the cycle time of the unit procedure yields the emission rate (in kmol/h) of a component during an operation. If several operations of a unit procedure contribute to VOC emissions, the total emissions from that procedure are combined and averaged over its cycle time.

A component's emission rate during an operation is averaged over the cycle time of the corresponding procedure that contains the operation and not over the duration of the operation.

10.3c Gas Sweep - Emission Model

This model accounts for emissions that are associated with sweeping a vessel with an inert gas (e.g., nitrogen). It is available in the Gas Sweep operation.

The model assumes that the sweeping gas leaves the system saturated with VOC vapor(s) at the exit (condenser) temperature. According to this model, the moles of a VOC component (i) emitted during a Gas Sweep operation are calculated using the following equation:

$$n_i = \frac{p_i(X_i)}{P - \sum_j X_j p_j} n_{inert} \qquad \text{eq. (10.22)}$$

where:

- n_i is the amount of the i-th component (in kmol),
- p_i is the vapor pressure of the i-th component at the exit temperature T (in Pa),
- p_j is the vapor pressure of the j-th component at the exit temperature T (in Pa),
- P is the pressure of the vessel during the operation (in Pa),

- X_i and X_j are the mole fractions of the i-th and j-th components, respectively, in the liquid mixture, and
- n_{inert} is the amount of inert gas flown through the vessel during the operation (in kmol).

If the vessel contains no liquid material but VOC vapors are present in the gas space, then the emission calculations are done using the following equation:

$$n_i = \frac{p_i (X_i)(V_r)}{RT}\left(1 - 0.37^N\right) \qquad \text{eq. (10.23)}$$

where:

- V_r is the vessel volume (in m^3),
- N is the number of volumes (multiple of vessel volumes) of sweeping gas, and
- T is the exit temperature.

Dividing n_i by the cycle time of the unit procedure yields the emission rate (in kmol/h). If several operations of a unit procedure contribute to VOC emissions, the total emissions from that procedure are combined and averaged over its cycle time.

A component's emission rate during an operation is averaged over the cycle time of the corresponding procedure that contains the operation and not over the duration of the operation.

10.3d Heating - Emission Model

This model accounts for emissions that are associated with heating a vessel that contains a mixture of volatile components. It is available in the following operations:

- Batch Heating,
- Batch Storage,
- Batch Solids Storage, and
- Solids Mixing.

During heating under constant pressure, the gas of the vapor space undergoes expansion and a fraction leaves the vessel through the vent. Further, during heating there is an increase in the vapor pressure of VOC compounds. The removed gas (due to expansion) is assumed to be saturated in VOC vapor(s) at the average vessel temperature.

The moles of a VOC component (i) emitted during any of the above operations are calculated using the following equation:

$$n_i = \frac{n_{inert}}{2}\left[\frac{(p_i)_{T_1} X_i}{P - \sum_j X_j (p_j)_{T_1}} + \frac{(p_i)_{T_2} X_i}{P - \sum_j X_j (p_j)_{T_2}}\right] \qquad \text{eq. (10.24)}$$

where:

- n_i is the amount of the i-th component (in kmol),
- T_1 is the initial temperature of the system (in K),
- T_2 is the final temperature of the system (in K),
- p_i is the vapor pressure of the i-th component at temperature T_1 or T_2 (in Pa),
- p_j is the vapor pressure of the j-th component at temperature T_1 or T_2 (in Pa),
- P is the pressure of the vessel during the operation (in Pa),
- X_i is the mole fraction of the i-th component in the liquid mixture, and
- n_{inert} is the amount of inert gas leaving the vessel during the operation (in kmol).

The amount of inert gas leaving the system is estimated using the following equation:

$$n_{inert} = \frac{V_r}{R}\left[\frac{P - \sum_j X_j \left(p_j\right)_{T_1}}{T_1} - \frac{P - \sum_j X_j \left(p_j\right)_{T_2}}{T_2}\right] \qquad \text{eq. (10.25)}$$

where:

- R is the ideal gas constant (8,314.5 J/kmol-K), and
- V_r is the volume of displaced gas (in m^3).

Following EPA guideline §63.1414 (Test methods and emission estimation equations, EPA 40 CFR Ch. I, 7-1-04 Edition), the above equations are used as shown if the final system temperature is lower than 50K below the mixture boiling point. Otherwise, the calculations are repeated with the temperature incremented from its initial value to 50K below the boiling point and then in 5K intervals up to its final value. The total heating emissions are then calculated as the sum of the estimated emissions in all incremental steps.

Dividing n_i by the cycle time of the unit procedure yields the emission rate (in kmol/h). If several operations of a unit procedure contribute to VOC emissions, the total emissions from that procedure are combined and averaged over its cycle time.

A component's emission rate during an operation is averaged over the cycle time of the corresponding procedure that contains the operation and not over the duration of the operation.

10.3e Gas Evolution - Emission Model

This model accounts for emissions from reaction operations that involve generation and release of an inert gas. It is available in the following operations:

- Batch Stoichiometric Reaction,
- Batch Kinetic Reaction,

- Batch Equilibrium Reaction,
- Batch Stoichiometric Fermentation,
- Batch Kinetic Fermentation,
- Perfusion Stoichiometric Fermentation,
- Batch Crystallization,
- Continuous Stoichiometric Reaction,
- Continuous Kinetic Reaction,
- Continuous Equilibrium Reaction,
- Continuous Stoichiometric Fermentation,
- Continuous Kinetic Fermentation, and
- Neutralization.

It is assumed that the gas that leaves the system is saturated with VOC vapor(s) at the exit temperature. The mathematical model is identical to the Gas Sweep model (see 10.3c Gas Sweep - Emission Model). Simply, the released gas plays the role of the sweeping gas.

10.3f Vacuum - Emission Model

In chemical processing, some operations (e.g., reaction, distillation, etc.) are carried out under vacuum. Under such conditions, a small amount of air leaks into the vessel and comes into contact with the contents of the vessel. The model assumes that the air that leaves the system is saturated with VOC vapor(s) at the exit temperature. The mathematical model is identical to the Gas Sweep model (see 10.3c Gas Sweep - Emission Model). Simply, the leaking air plays the role of the sweeping gas. The leak rate must be specified by the user.

10.3g Drying - Emission Model

Wet cakes recovered from filtration and centrifugation operations frequently contain solvents in their interstitial space. The drying of such cakes results in emissions. The emission calculations are based on simple material balances (inlet minus outlet flow). By default no control device is associated with drying operations. If a control device (e.g., condenser, absorber, activated carbon column) is required, it should be added explicitly using a separate unit and directing the vent streams of the dryer to the control device.

10.4 EMISSIONS REPORT (EMS)

The Emissions Report (EMS) presents information on air pollutant flow from the various procedures of a process. To generate this report, click **Emissions (EMS)** on the **Reports** menu; for more details on the contents of this report, see 12.6b Emissions Report (EMS).

10.5 EMISSION LIMITS

You can set emission limits for the various pollutant categories, except for volatile organic compounds (VOCs) through the Emission Limits Dialog. To access this dialog, do one of the following:

- click on an empty area on the flowsheet and then click **Process Options ▸ Preferences ▸ Emission Limits** on the **Edit** menu, or
- right-click on an empty area on the flowsheet to bring up its context menu and click **Preferences ▸ Emission Limits**.

The emissions of VOC components are calculated by the program based on the composition of the various vent (emission) streams. The Emissions Report (EMS) will include warnings if the accumulated emissions for any of the categories included in the above dialog exceed the specified limit.

Through the same dialog you can introduce four additional used-defined pollutant categories and specify their limits. Once a user-defined pollutant category has been introduced, you can classify any component present in this process file as contributing to that category; for more details, see 3.1e Pure Component Properties.

11

DEBOTTLENECKING

Throughput analysis and debottlenecking studies are very important when developing a new process or even when improving existing recipes. This chapter will explain all the terms and present the methodology used when performing throughput analysis and debottlenecking studies. Also it will describe the throughput analysis charts which are relevant to this topic. This chapter includes the following sections:

- Definitions & Theory of Throughput Analysis
- Scale-up (or down) Process Throughput
- Throughput Analysis Report

11.1 DEFINITIONS & THEORY OF THROUGHPUT ANALYSIS

The *batch throughput* (or *batch size*) of a batch manufacturing facility corresponds to the amount of material that is processed per batch. The *annual* (or *campaign*) *throughput* of a batch manufacturing facility corresponds to the amount of material that is processed per year. It is calculated as the batch throughput times the number of batches that can be processed per year:

$$\begin{matrix}\text{Annual}\\ \text{Throughput}\end{matrix} = \begin{matrix}\text{Batch}\\ \text{Throughput}\end{matrix} \times \begin{matrix}\text{Number of}\\ \text{Batches per Year}\end{matrix} \qquad \text{eq. (11.1)}$$

Therefore, we can increase the annual throughput by either increasing the batch throughput, or the number of batches per year, or both. In our effort to increase annual throughput we run into

bottlenecks that are either related to equipment or resources (e.g., utilities, labor, demand for raw materials).

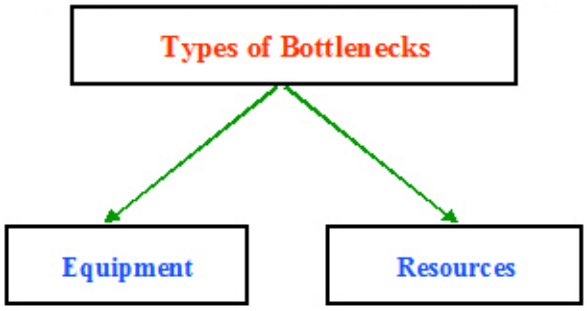


Figure 11.1: Type of Bottlenecks.

The equipment or resource that limits the number of batches per year is the *scheduling* (or *time*) *bottleneck*. The equipment or resource that limits the batch throughput is the *batch size bottleneck*. The equipment or resource that limits the annual throughput is the *throughput bottleneck*. Either the time or the batch size bottleneck is also the throughput bottleneck.

Please note that for a batch process the batch size and the number of batches per year are interdependent. More specifically, as the batch throughput is increased (operating closer to the maximum), the cycle time of most procedures will increase resulting in longer recipe cycle times and fewer batches per year. Consequently, the maximum annual plant throughput cannot be simply set equal to the maximum batch size times the maximum number of batches per year. Instead, it can be calculated in an iterative way by gradually increasing the batch size and letting SuperPro Designer calculate the corresponding maximum number of batches.

11.1a Identifying Equipment Time (Scheduling) Bottlenecks

Information on the equipment scheduling bottleneck is provided on the Recipe Scheduling Information Dialog (see Chapter 7 (Scheduling)). The same information can be visualized graphically on the Equipment Occupancy Chart (see 6.2a Equipment Occupancy Chart). The scheduling (or time) equipment bottleneck is the piece of equipment that has the longest cycle time. This piece of equipment determines the minimum time between consecutive batches (also known as minimum recipe cycle time) and consequently the maximum number of batches per year. For main equipment items that are shared by multiple procedures, their cycle time is set equal to the time interval between the start of the first procedure that is hosted by the equipment to the end of the last procedure that is hosted by the same equipment. Please note that resources also can become time bottlenecks (see 11.1d Resource Bottlenecks).

11.1b Identifying Equipment Size and Throughput Bottlenecks

The batch size bottleneck can be identified by considering the capacity and time utilization of each equipment item.

EQUIPMENT CAPACITY UTILIZATION

The *equipment capacity* (or *batch size/throughput*) *utilization* represents the percentage of equipment capacity that is utilized during a certain unit procedure. For instance, if a piece of equipment that can process up to 100 kg/h of a certain material is operated at a rate of 80 kg/h,

its equipment capacity utilization will be 80%. If a piece of equipment is of vessel type, its capacity utilization can be defined based on the ratio of actual and maximum liquid levels for a certain operation:

$$\text{Equipment Capacity Utilization} = \frac{(\text{Actual Liquid Level})}{(\text{Max Liquid Level})} \times 100 \qquad \text{eq. (11.2)}$$

Figure 11.2 illustrates this in detail. The equipment capacity utilization of a unit procedure corresponds to the maximum equipment capacity utilization among all operations of that unit procedure. The cyclical equipment with storage capacity that has the highest capacity utilization determines the maximum batch size and is therefore the batch size bottleneck.

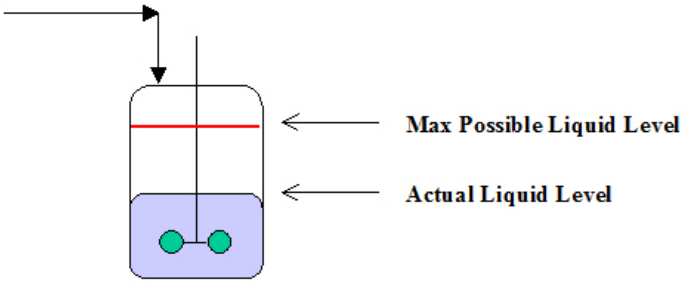


Figure 11.2: Capacity Utilization

EQUIPMENT UPTIME

The *equipment uptime* represents the percent of overall operating time that a certain piece of equipment is occupied. For batch processes, the equipment uptime can be defined as follows:

$$\text{Equipment Uptime} = \frac{(\text{Total Time Equipment is Utilized per Batch})}{(\text{Recipe Cycle Time})} \times 100 \qquad \text{eq. (11.3)}$$

The *recipe cycle time* is the time interval between consecutive batches. If a piece of equipment is used by multiple procedures (in a batch plant), the equipment uptime accounts for the overall (of all procedures) utilization in time.

Many procedures have uptimes (as well as cycle times) that are proportional to the amount of material processed per cycle. For example, if you have a disk-stack centrifuge that processes material in a continuous fashion without accumulating anything and double the batch volume, the uptime of the centrifuge will also double. Equipment items of this type usually operate at 100% capacity utilization and changes in batch size only affect their uptime. This is an important point to understand; just because a piece of equipment is listed as having 100% capacity utilization, it not necessarily the throughput bottleneck. For this reason, a combined utilization is also calculated as described below.

COMBINED UTILIZATION

The *combined utilization* of a unit procedure is calculated as its equipment capacity utilization times its equipment uptime. To have a combined utilization of 100%, the procedure's equipment would have to be run at full capacity and its cycle time would have to be the same as the recipe cycle time. The procedure with the highest combined utilization is identified as the throughput bottleneck for a process in the Throughput Analysis: Utilization Factors Chart. An example of this chart is shown in Figure 11.3. This chart displays the percent equipment capacity, time and combined utilization for each unit procedure-equipment combination in a process. This chart is generated by selecting **Charts ▸ Throughput Analysis ▸ Utilization Factors** from the main menu of the application. By default, only unit procedures whose equipment is in Rating mode (i.e., the equipment size is user-defined) are included. However, you can choose to allow (if so desired) to display equipment in Design mode as well by visiting the Style for Throughput Utilization Chart Dialog (right-click on the chart and select **Edit Style** on the context menu that appears).

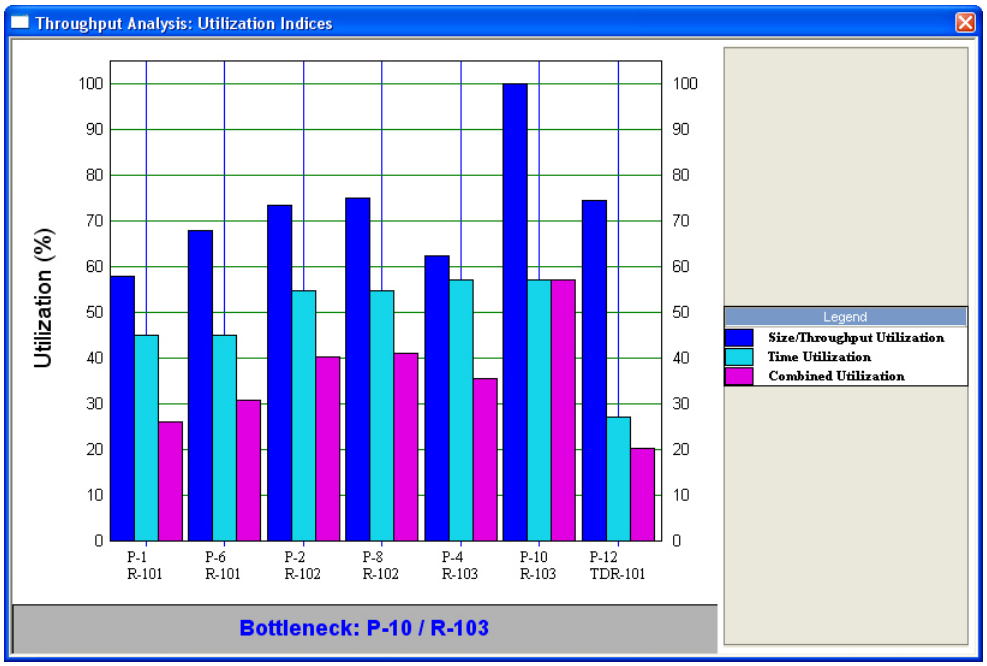


Figure 11.3: Throughput Analysis: Utilization Factors chart.

For this example, procedure P-10 that utilizes vessel R-103 has the highest combined utilization and is therefore identified as the throughput bottleneck based on this criterion. This methodology points in the right direction regarding bottleneck identification, but it cannot guarantee identification of the right bottleneck when cyclical procedures are included in the process. Cyclical procedures (i.e., procedures that go through cycles of activities, such as batch chromatography steps) impose constraints on time utilization and may lead to situations where the true throughput is a procedure that does not have the highest combined utilization. For instance, if the recipe cycle time of a batch process is 100 hours, and a reaction step in a vessel takes 60 hours, in a regulated environment where batch integrity is maintained (that's the case with the pharmaceutical industry), the reaction vessel can have a practical maximum uptime of

60%. If the specific vessel operates at full size utilization, it will be the throughput bottleneck even if some other equipment has a higher combined utilization.

11.1c Potential Maximum Throughput Size

A better way of identifying throughput bottlenecks is by calculating the *Potential Maximum Throughput* (PMT) of each procedure. For procedures that have cycle times proportional to batch size (e.g., disk-stack centrifugation, pumping, etc.), the PMT is calculated by assuming 100% equipment capacity utilization and 100% uptime. For procedures whose cycle times are not proportional to their throughputs (e.g., vessel procedures, chromatography, etc.), their PMT is calculated under conservative, realistic, and theoretical assumptions for their uptime:

1. In the *conservative* case, the equipment uptime is kept the same as its current uptime.
2. In the *realistic* case, the equipment uptime is set to correspond to the highest number of complete cycles that can be performed in that piece of equipment within the time window of the current recipe cycle time.
3. In the *theoretical* case, the equipment uptime is assumed to be at 100%. This would require mixing of partial lots of product, which typically is not an option in the regulated industries (e.g., pharmaceutical industry).

The equipment capacity utilization is assumed 100% in all the cases. This is illustrated in Figure 11.4 below. In this figure, EPBT (Equipment Potential Batch Time) corresponds to 100% equipment uptime.

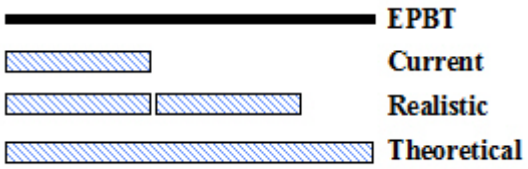


Figure 11.4: Potential batch size.

The objective is to identify the TRUE throughput bottleneck based on the realistic scenario. The conservative scenario corresponds to the case where we operate all the equipment items at

100% capacity utilization but without making any changes in the number of cycles per batch. Figure 11.5 shows the Throughput Analysis: Batch Size/Throughput Potential Chart (the PMT

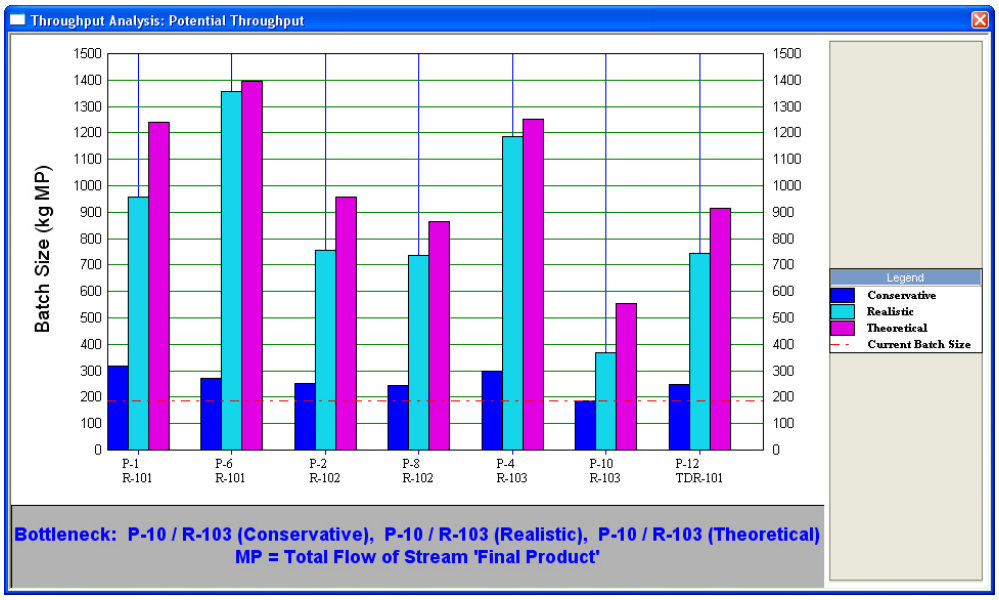


Figure 11.5: Throughput Analysis: Potential Throughput chart.

chart) for a process. This is the same process for which the Utilization Factors chart was shown previously in Figure 11.3. The PMT chart is generated by selecting **Charts ▸ Throughput Analysis ▸ Batch Size Potential** from the main menu of the application. For this example, it can be seen that all three indicators identify the unit procedure-equipment combination P-10 / R-103 as the bottleneck based on this approach as well. That's a good sign that indeed this is the true bottleneck of this process.

Equipment can be excluded from throughput analysis by visiting the Equipment Data Dialog: Throughput Tab and checking the 'Omit from Throughput Analysis' option. Then the equipment will not be displayed in any Throughput Analysis Charts (Utilization, Potential). In particular if an equipment is omitted from scheduling calculations it is also omitted from throughput analysis.

You can change the appearance of the PMT chart by visiting the Style for Throughput Potential Chart Dialog (right-click on the chart and select **Edit Style** on the context menu that appears).

11.1d Resource Bottlenecks

Resources can become size and time bottlenecks when their average or instantaneous demand exceeds their average or instantaneous capacity, respectively. For instance, Figure 11.6 below shows the demand for labor as a function of time for three consecutive batches of a process. For short periods of time, there is a need for up to eight operators. If seven (red line) is the maximum number of operators that can be available at any time, then, certain operations will have to be delayed to accommodate that constraint. That delay of operations may increase the recipe cycle time and reduce the maximum number of batches per year and therefore become the new time bottleneck.

The current version of SuperPro Designer does not identify resource time bottlenecks. However, it calculates and displays the demand for any resource (e.g., raw materials, heating/cooling utilities, power, and labor) and enables the user to visualize and interactively eliminate potential resource bottlenecks. In SchedulePro, however, the user may specify a maximum for each resource and the scheduling algorithm will automatically delay the execution of certain operations in order to meet those constraints.

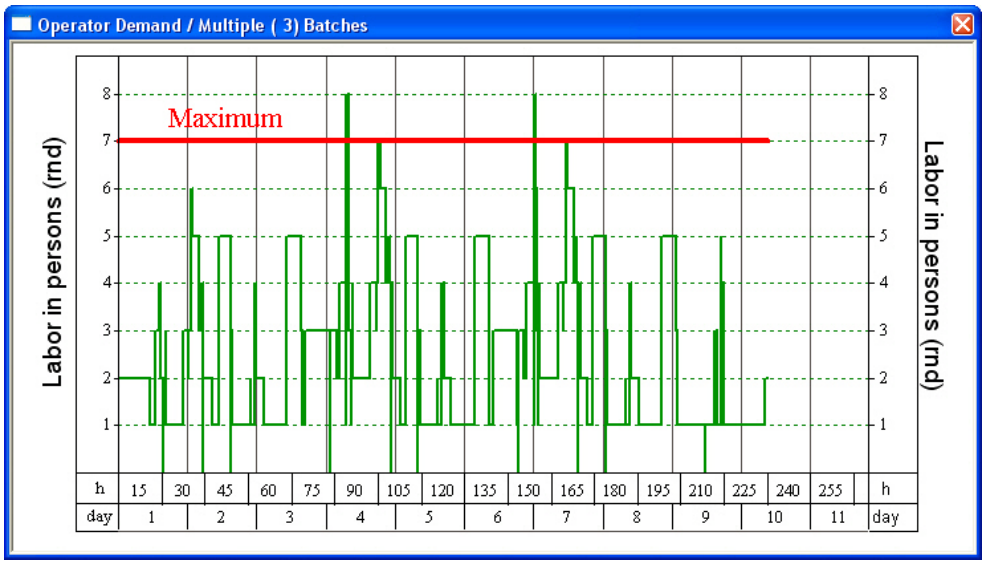


Figure 11.6: Resource demand chart.

For more information on resources and resource time charts, see Chapter 6 (Resources).

11.1e Using Multiple Equipment Sets in Staggered Mode

When a specific piece of equipment becomes the overwhelmingly dominant scheduling bottleneck in a recipe, in other words, when its occupation time (per batch) exceeds by far any other equipment in the recipe, thereby leading to large plant cycle times, it is worthwhile to consider using extra pieces of equipment operating in staggered mode to effectively reduce the plant's cycle time.

For instance, consider a recipe involving a fermentation procedure that lasts one week (or 168 hours) followed by a downstream processing sequence where the longest procedure doesn't exceed 48 hours. If you restrict yourself operating with a single fermentor vessel, then you are forced to start a batch once every 168 hours, which is the recipe cycle time in this case. This is depicted in the Equipment Occupancy Chart of Figure 11.7. Clearly, the scheduling bottleneck

(the equipment with the longest cycle time) in this case is the fermentor vessel FR-101; for more details on this chart, see 7.6 The Equipment Occupancy Chart (EOC).

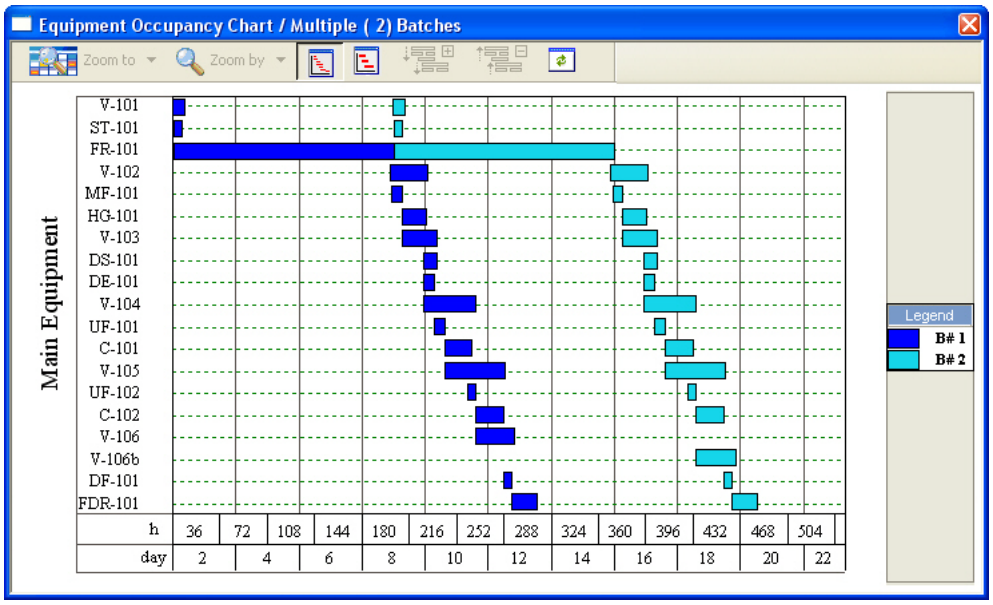


Figure 11.7: Equipment Occupancy Chart of an example recipe involving a long fermentation procedure.

However, if you could use 6 additional fermentors (of the same or larger size) and operate them in staggered mode, i.e., start them at 48 hours apart, then, you could reduce the recipe's cycle time to 48 hours, thereby increasing your annual throughput by a factor of 7.

In SuperPro Designer, you can specify *extra sets* (M) of equipment in staggered mode (i.e., out of phase) for an equipment resource. A set consists of a *number of units* operated in parallel (i.e., simultaneously). This is either specified (in Rating Mode) or calculated (in Design Mode). Consequently, the actual number of units represented by an equipment resource will be equal to the total sets (M+1) times the number of units (N).

Specifying extra sets of equipment in staggered mode for an equipment resource in SuperPro Designer is very simple. Just bring up the Equipment Data Dialog: Equipment tab of a unit procedure, set the 'Stagger Mode' option to 'On', and type in the number of extra sets of equipment that you wish to use in association with that unit procedure. For instance, in the example mentioned earlier in this section, you would type '6' as the extra sets in staggered mode and click **OK** to close the dialog. Then, you should redo the M&E Balance calculations and observe the new value of the recipe's cycle time.

The Equipment Occupancy chart of the recipe after 6 extra sets of fermentors are specified in staggered mode is shown in Figure 11.8. Since staggering M extra pieces of equipment in that unit procedure essentially reduces the participation of that unit procedure to the recipe cycle time by a factor equal to M+1, and unless another piece of equipment becomes the scheduling time bottleneck, the recipe cycle time will be reduced by just as much. Of course, if another unit procedure (e.g., a long chromatography step or storage unit) becomes the time bottleneck, then the reduction of the recipe cycle time will be determined by the cycle time of that unit procedure. This is the case for the example presented above, in which the blending tank V-105

is now the scheduling bottleneck (the corresponding unit procedure carried out in that equipment has the longest cycle time).

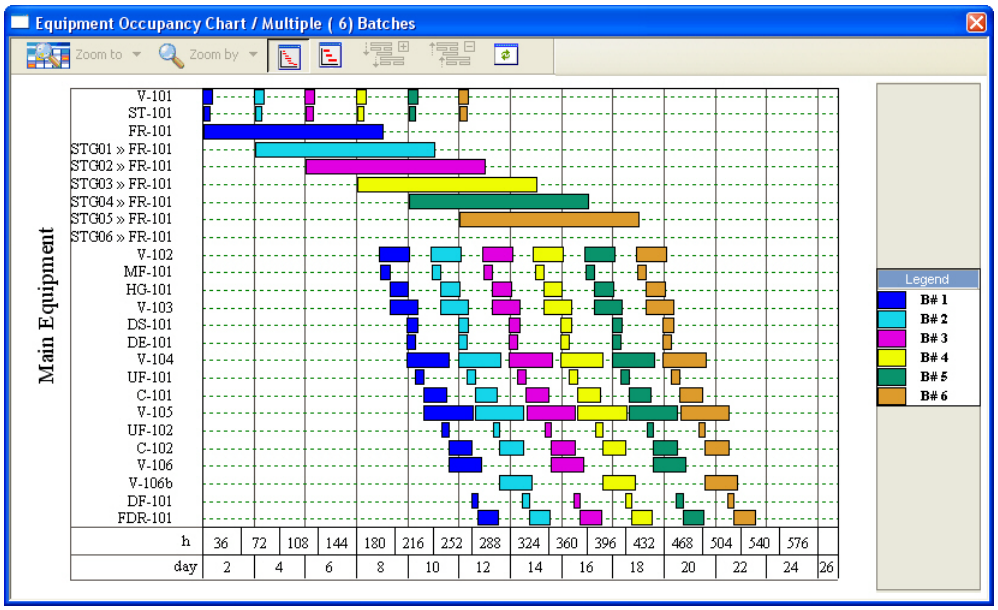


Figure 11.8: Equipment Occupancy Chart of the example recipe after 6 extra sets of fermentors are specified in staggered mode.

Even though users do not name the staggered equipment, SuperPro Designer will automatically generate names for them that will be used when presenting the Equipment Occupancy chart. The names of the staggered equipment are created by using as starting root the name of the main equipment (as set by the user on the recipe) and adding in front of that name the string "STG01>>", "STG02 >>", etc. to indicate the first, second, etc. additional pieces of equipment utilized in staggered mode (see chart above).

For more information on equipment sizing, please see 6.1a Equipment Sizing (Design vs Rating Mode). For more information on equipment staggered mode, please see 6.1c Staggered Mode.

11.2 SCALE-UP (OR DOWN) PROCESS THROUGHPUT

After a process description is completed and the mass and energy balances are done satisfactorily, oftentimes, you need to try and see how the process would behave if you scaled it up (or down) by a factor. In order to do that, you must visit all process input streams and adjust them by the scale-up (or scale-down) factor, and re-run the simulation. SuperPro Designer facilitates this process by offering you the option to do all this in just one step: All you have to do is select the **Tasks ▸ Adjust Process Throughput** option from the main menu of the

application. The Process Throughput Adjustment Dialog dialog shown in Figure 11.9 will appear.

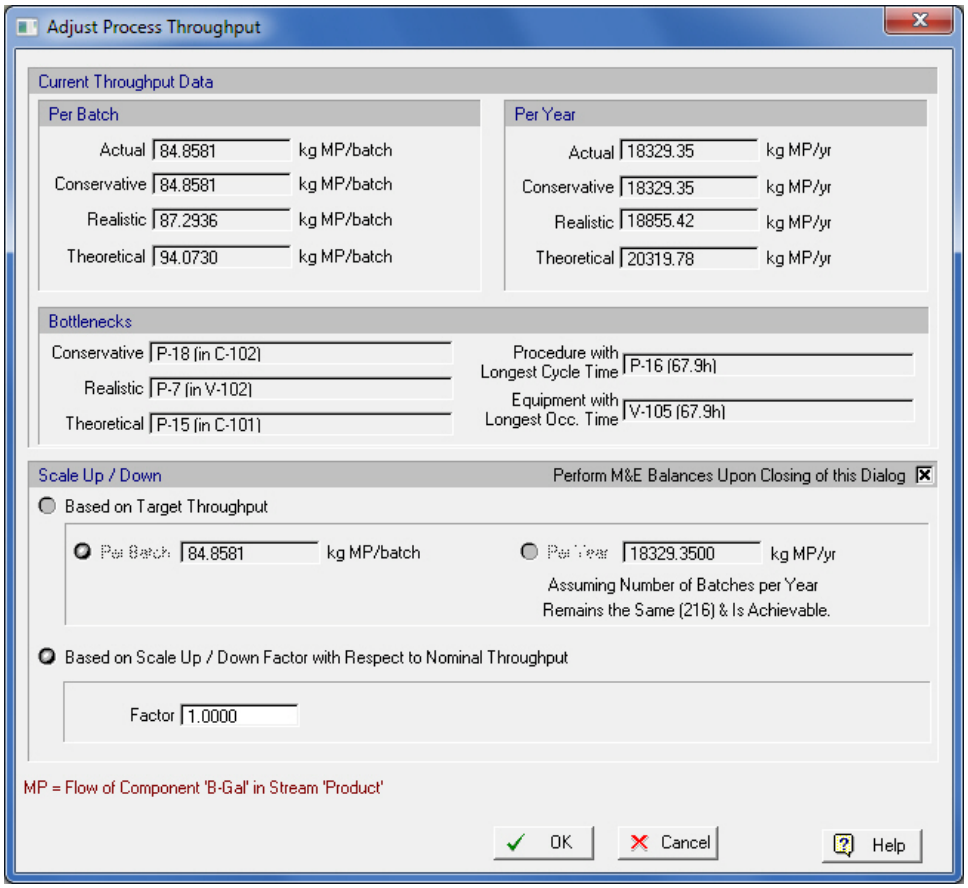

Adjust Process Throughput
Current Throughput Data
Per Batch
Actual 84.8581 kg MP/batch
Conservative 84.8581 kg MP/batch
Realistic 87.2936 kg MP/batch
Theoretical 94.0730 kg MP/batch
Per Year
Actual 18329.35 kg MP/yr
Conservative 18329.35 kg MP/yr
Realistic 18855.42 kg MP/yr
Theoretical 20319.78 kg MP/yr
Bottlenecks
Conservative P-18 (in C-102)
Realistic P-7 (in V-102)
Theoretical P-15 (in C-101)
Procedure with Longest Cycle Time P-16 (67.9h)
Equipment with Longest Occ. Time V-105 (67.9h)
Scale Up / Down
Perform M&E Balances Upon Closing of this Dialog
Based on Target Throughput
Per Batch 84.8581 kg MP/batch
Per Year 18329.3500 kg MP/yr
Assuming Number of Batches per Year Remains the Same (216) & Is Achievable.
Based on Scale Up / Down Factor with Respect to Nominal Throughput
Factor 1.0000
MP = Flow of Component 'B-Gal' in Stream 'Product'
OK
Cancel
Help

Figure 11.9: The Process Throughput Adjustment Dialog.

From the above dialog, you can simply type in the scale-up (or scale-down) factor and then SuperPro Designer will automatically increase (or decrease) all input stream flowrates by that factor. Alternatively, if you don't wish to have all input streams scaled-up (or down) by the same factor, you can select the second option, and supply such a factor for each input stream.

Typically, after you have scaled up (or down) the process inputs, you must re-solve the M&E balances. If several pieces of equipment have their sizes specified (i.e., they are in rating mode), a scale-up adjustment may result in a process throughput that exceeds their capacity. In

that case, the program will display appropriate warning messages and provides instructions on how to fix the problem.

For a batch process that has not been designed and built yet, a throughput adjustment is equivalent to a batch scale-up or scale-down. For an existing batch plant, with fixed equipment sizes, a scale-up action usually increases the minimum effective plant batch time and decreases the maximum number of batches per year. In other words, the number of batches per year decreases, but the amount produced per batch increases. As a consequence, there is an optimum value of batch throughput that corresponds to maximum annual throughput.

For detailed definitions of the terms **Conservative**, **Realistic** and **Theoretical** throughputs, see 11.1c Potential Maximum Throughput Size.

11.3 THROUGHPUT ANALYSIS REPORT

The Throughput Analysis Report includes the information of the Throughput Analysis (Utilization Factors and Batch Size Potential) charts in tabular format along with additional details regarding procedure/equipment utilizations and potential batch sizes. The report can be generated by selecting **Reports ▸ Throughput Analysis (THR)** from the main menu of the application. A throughput debottlenecking exercise is described in the 'Examples \ SynPharm' directory of SuperPro Designer.

- For information on the definition of the terms used in the reports, see 11.1 Definitions & Theory of Throughput Analysis.
- For information on the sections and structure of the report itself, see 12.5 Throughput Analysis Report (THR).
- For information on changing the format / contents of the report, see Report Options Dialog: Throughput Analysis Tab.

12

REPORTS

There are hundreds, possibly thousands of numbers (depending on the size of your process description) that are calculated after the simulation is performed (M&E balances) and the economic calculations are finished. The results cover a wide span of interests regarding the performance of the process: batch (or throughput) size, annual throughput, yields, material (or any other resource) consumption levels, scheduling constraints, economic viability, environmental impact assessment, just to name a few. It would be very difficult to search into all the process objects (procedures, operations, equipment, etc.) and collect all the pertinent numbers to get answers on typical questions that users may have regarding a process. There are many user interfaces that interactively present partial views of those results on the screen in the form of charts, tables, etc. but the scope of such views is limited:e.g. you can view the contents of a single equipment or the consumption chart for a selected material. SuperPro Designer comes to the help of the user by collecting all the relevant numbers and presenting them in the form of reports. There are several reports generated by the application, each focusing on a different group of issues. The reports are generated (upon request using appropriate menu calls) and saved in a temporary file just so that they can be presented to the user. The file format of the report can be chosen by the user (e.g. 'pdf', 'rtf', 'html', etc.) and its choice dictates the viewer application employed to present the report on the screen. Each time you request a report the previous version is deleted. If needed, you can request to have a given set of report(s) preserved in a location and not overwritten by the application the next time they are generated (see Create and Save Multiple Reports Dialog). The following reports are currently generated:

- Material & Stream Report (SR)
- Economic Evaluation Report (EER)
- Cash Flow Analysis Report (CFR)
- Itemized Cost Report (ICR)
- Throughput Analysis Report (THR)
- Environmental Impact Report (EIR)
- Emissions Report (EMS)
- Equipment Report (EQR)
- CIP & SIP Report (CSR)
- Input Data Report (IDR)
- Custom Excel Report

The content of each report mentioned above is preset but users may include or exclude some of the sections or paragraphs if needed (see Report Options Dialog). Finally, there's another report (Custom Excel Report) which is only generated in MS-Excel® native format, and whose

contents are not focused on any particular group of issues but they can be chosen by the user from a list that covers all aspects of the results: stream flows, equipment contents, economic figures, scheduling data, consumption charts, etc. The Custom Excel Report can be used to quickly generate content that may be suited for users who want to see in a single file perhaps a collection of performance indicators for the process in an arrangement that the application does not currently support in the form of a standard report.

12.1 GENERATING AND VIEWING REPORTS

The program allows you to generate and view the following reports:

- Material & Stream Report (SR)
- Economic Evaluation Report (EER)
- Cash Flow Analysis Report (CFR)
- Itemized Cost Report (ICR)
- Throughput Analysis Report (THR)
- Environmental Impact Report (EIR)
- Emissions Report (EMS)
- Equipment Report (EQR)
- CIP & SIP Report (CSR)
- Input Data Report (IDR)
- Custom Excel Report

Each of the above reports can be generated (and viewed) in any of the following formats:

Format	Viewer Application
Preview	A proprietary formatted report is generated and can be viewed (but not edited) by a viewer application provided with the software. This choice yields nicely formatted reports generated very fast.
MS-Excel® (Fully-Formatted)	MS-Excel® is required to be installed on your PC in order to be able to view a report generated in this format. Columns may be appropriately sized and feature appropriately formatted headers. The file generated can also be edited (if needed).
MS-Excel® (Unformatted)	MS-Excel® is required to be installed on your PC in order to be able to view a report generated in this format. The data are only included in the file and no formatting has been applied. It may be preferred if the exported data are formatted later (in the destination file) using MS-Excel®'s richer toolset (file is editable by the host application).
PDF	Adobe's PDF Reader® is required to be installed on your PC in order to be able to view a report generated in this format (free utility that can be downloaded from Adobe's website. The file is not editable (unless users own Adobe's Acrobat® or Acrobat Pro®).

HTML	An Internet browser (like Internet Explorer®) must be installed on your PC in order to be able to view a report generated in this format. The file is not editable unless opened by an HTML editor application.
RTF	Rich Text Format (rtf) is supported by several editors (incl. MS-Wordpad® that is part of MS-Windows®, or MS-Word®, that is part of MS-Office®). The report file can be edited when viewed by any of the aforementioned viewer applications.
ASCII Text	Any ASCII text editor (e.g any of the applications mentioned above or even MS-Notepad® that is part of MS-Windows®) can be used to open and edit the report. Even though the same information (as any of the other report formats) is included, the results are not formatted nor arranged in any that are easily viewable by the user. This format may be appropriate if users need to export the numbers in a format that can be parsed by another application.
XML	Any XML editor or any other third-party program that can parse and incorporate XML-based content. Users should not opt for this format when they wish to view the results with a regular editor.

You can choose the format for the reports from the Report Options Dialog: General (Default) Tab (part of the Report Options Dialog that appears when you select **Reports ▸ Options** from the main menu of the application). From the same dialog you may set other choices that apply to either all reports or just to a particular report. The report-specific options are displayed on the corresponding tab. The common options are presented in the 'General' tab.

The Custom Excel Report can only be created in the Excel (Fully Formatted) format.

You can request to generate and view a report by selecting the **Reports ▸ <Report-Name>** option from the application's main menu. Before creating a report file, the program will check to verify that all simulation results and cost items are up-to-date. If not, then it will ask the user's permission to redo the calculations prior to generating the report. Then, the application will gather all the relevant data and generate a temporary file that will be saved in the same location (folder) as the process file, and its name will be assigned automatically based on:

- The name of the process file(e.g. "projectX.rv1.spf")
- The type of report chosen (e.g., stream report (SR), or economic evaluation report (EER), etc.), and
- The format chosen for the report (determines the file extension 'pdf', 'xls', etc.)

Since the name and location of the process file is used to auto-generate the name (and location) of every process report, the application cannot generate any report unless the process you are currently working has been saved on the disk at least once.

Since the same exact file name and location will be used every time you pick a **Reports ▸ <Report-Name>** option to generate a given report, you must make sure the previous (older) version of the report file is not still shown by the host application (e.g. MS-Excel®, MS-Word®, etc.). If it is, SuperPro Designer will generate an error: "The report file <file name> cannot be created on disk. The file may be in use by another application...". If the report generation completed successfully, a new version of the report file will be generated (overwriting a previous version without user warning) presented for viewing by the appropriate viewer. If you want to preserve one or more reports and protect them from being overwritten the next time the same report generation command is issued, then you should use the **Reports ▸ Create and Save As** option (see 12.12a Create and Save Multiple Reports Dialog).

If you request to view a given report (e.g. the economic evaluation report) and the report file already exists (since the prior call to generate the EER) and no variables affecting any of the economic calculations has changed, then the application will simply present the previously generated file without recreating it. However each report is re-created all the time if it hasn't been created before in the current session (regardless of possible input changes that may or may not have been recorded). The program will notify the user about the fact that some of the reports contents may be outdated, and present a message like: ("Data affecting the simulation results have changed. Solve M&E balances first? Yes/No?" Regardless of what the user selects (Yes or No) the program will create a new report; if the user had opted to re-do the M&E calculations then new numbers will be created; if the user selected 'No' then the report will be re-created using the (possibly outdated) results.

If you wish to open any report file, not necessarily the standard reports associated with the process file currently open by the application, then you can select the **Reports ▸ View Any Report** option from the main menu. In the file selection dialog that will appear, locate the report file that you wish to open and click on **OK**. Depending on the format of the report file you selected, the appropriate report viewer will be called upon to display the report contents.

12.2 GENERAL (DEFAULT) REPORTS OPTIONS

There are several attributes that are common to all reports and can be set from Report Options Dialog: General (Default) Tab and shown in Figure 12.1 below. The Report Options Dialog can be opened when you select **Reports ▸ Options** from the main menu of the application. These common settings have to do with:

- The format of the report: '.LL' (default), 'pdf' (Adobe), 'xls' (MS-Excel), etc. For a complete list of available formats, see 12.1 Generating and Viewing Reports.
- Pagination / Page Header & Footer Contents: Specify (if needed) to display special information on the header and/or footer area of each page of the reports: for example, you can display the name of the report file, or the date, or a special bitmap (company log) etc.
- Include / exclude charts in the reports (in report sections where available).
- Indicate how you wish to have the component names be presented on the report. Typically the 'local name' is used, but you can substitute or expand the name to include other names (e.g. trade name, or company name).

- Numerical format options: specify what to use for the thousands indicator (esp. important for the economic reports) and how many decimal points you wish to be used when displaying several key physical quantities (in all reports): e.g. mass flows (on an hourly or yearly basis), mass/mole compositions, temperatures, pressures, concentrations, densities, etc.

Note that even though all the feature selections made on this page of the report options dialog are used by all report types (EER, ICR, etc.) it is possible, if need be, to overwrite the defaults for just one of the reports (e.g. the economic evaluation or EER report).

All economic reports will present income and cost figures in US$ (by default). However, you can change the currency used by the application when reporting or soliciting cost- or income-related parameters for a specific process (see 9.8 Currency). If the currency you want is not listed, then you can introduce it in the currencies databank (see 15.12 Currencies Databank). As soon as you make your new currency selection, all economic figures will be converted based on the exchange rate kept by the document, and all economic reports from then onwards will show their figures in the new currency.

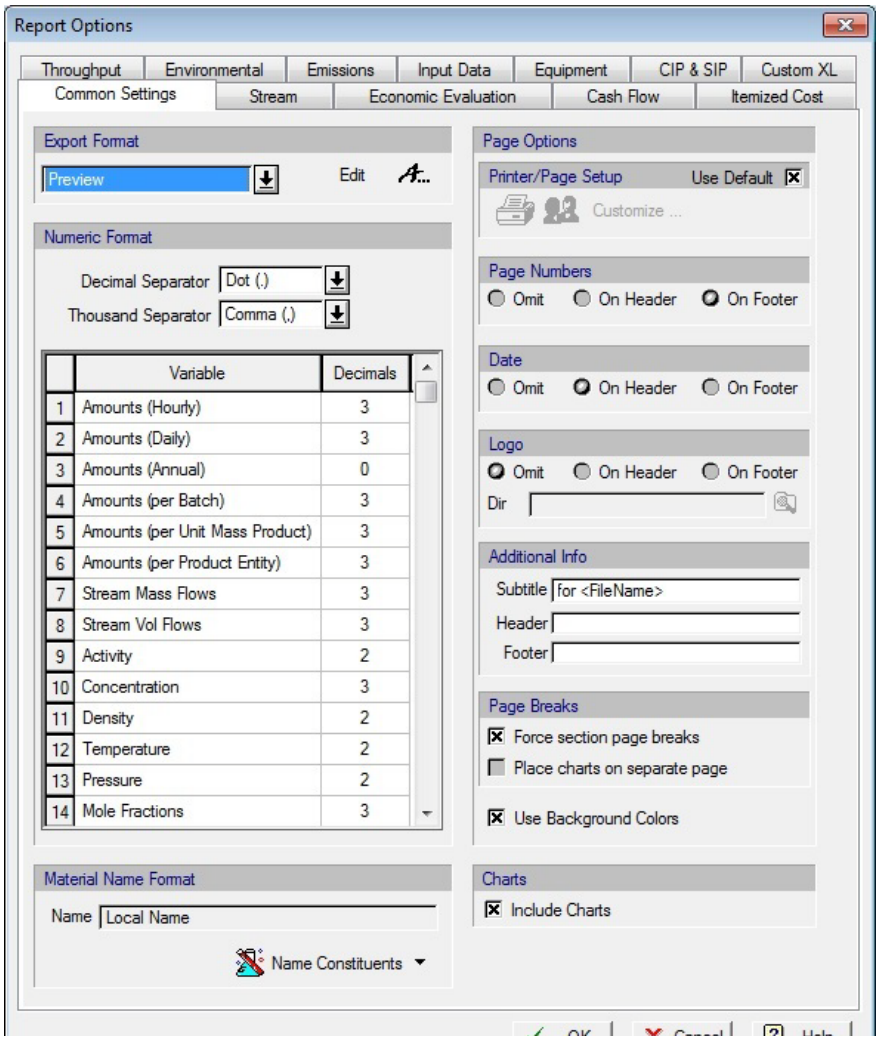


Figure 12.1: Report options dialog: 'General (Default)' options tab.

▶ To overwrite the default general settings for a specific report...

1. Open the Report Options Dialog and select the tab that corresponds to the report whose settings you wish to change.
2. Locate the 'General Options' box (at the top left corner of the tab); instead of accepting 'Use Defaults' switch to 'Use Custom' and notice that the **Customize** button (Customize...) becomes active.
3. Click on the **Customize** button (Customize...) to bring up the a dialog that displays all the common settings for all reports, with the choices currently based on the common (default) choices. Make any changes that you want to apply to this report only, and click on

OK. For more information on the default settings see Report Options Dialog: General (Default) Tab.

12.3 MATERIAL & STREAM REPORT (SR)

The materials and streams report (SR) can be generated by selecting **Reports ▸ Materials & Streams (SR)** from the main menu. It contains the following sections:

1. Overall Process Data (always)
2. Material Requirements
3. Stream Details
4. Overall Component Balance
5. Equipment Contents

The first section of the materials & streams report (overall process data) is always part of the SR contents. All other sections may be included or excluded from the report (at the user's discretion and using settings displayed in the Report Options Dialog: Stream Tab)

SR: MATERIAL REQUIREMENTS SECTION

This section of the report presents a cumulative account as well as detailed (section-by-section or even procedure-by-procedure) analysis of material requirements for the process. When you request to see material demand broken down per material and per procedure, please be advised that when dealing with a rather large process (over a hundred steps) this section can become excessively large. Opt to see the demand broken down by section instead. The material demand may include material used as 'Raw Material' only (i.e. part of input stream classified as 'Raw Materials', or material consumed in any other possible mode (see 6.5a Entering Material Consumption Classification).

SR: STREAM DETAILS SECTION

In this section, the report will present for each stream the following properties:

(a) Name
(b) Source Unit Procedure (or INPUT if it is an input stream)
(c) Destination Unit Procedure (or OUTPUT if it is an output stream)
(d) Activity (U/ml)
(e) Temperature (°C)
(f) Pressure (bar)
(g) Density (g/l)
(h) Component Weight Percentages
(i) Component Flowrates
(j) Total Mass or Molar Flowrate (kg/h or kg/batch)
(k) Total Volumetric Flowrate (m3/h or m3/batch)

You can instruct SuperPro Designer to exclude from the SR report streams with zero flowrates or to exclude from listing in the composition list ingredients with zero mass fraction. Also, you can directly edit the list of streams included in the 'Stream Section' of the SR, by visiting the Report Options Dialog: Stream Tab (top right box, 'Stream Section').

SR: OVERALL COMPONENT BALANCE SECTION

In this section of the SR report the application will present an aggregate amount for each component that enters or leaves the process (by any means). Material present as equipment content (at the beginning and the end of the batch) will also be included in the totals, even though the next section is dedicated exclusively on equipment contents.

Besides the standard form of consuming material through input streams (and exit the process via process output streams), sometimes material enters the process without the presence of an input stream (and leaves the process without the presence of an output stream). For example, several operations may engage the use of some material agents directly from their i/o simulation dialogs (e.g. CIP, Gas Sweep, etc.) For most of these operations the same amount of material that enters the process also leaves the process (during the same operation) thus not affecting the overall mass balance. There are some (rare) exceptions: for example, it is possible for the cleaning agent set at a CIP step to take with it any left-over vessel contents (if so specified at the operation's i/o simulation dialog); also, the sampling operation may actually remove a (small) amount of material from the vessel contents (even though there's no stream shown to hold it).

At the end of the overall mass balance section, the sum of all material entering and leaving the process, as well as their difference is displayed at the bottom right corner. Since no mass is lost in any of the unit operations supported by the program (no mass to energy conversion anywhere) *the difference between the total amount of materials entering and leaving the process should always be zero*. In processes with recycle loops, it is possible to encounter situations where that difference between total input and output is non-zero (usually a small number). This is typically attributed to round-off errors during the loop convergence as part of the simulation calculations. If the scope for your simulation demands more accuracy, then it is recommended to tighten up the convergence criterion for recycle loops (i.e., reduce the allowed tolerance) and/or switch from total flow based convergence to component-flow-based convergence (see Recycle Loop & Tear Stream Options Dialog or select **Recycle Loop & Tear Stream Options** from the flowsheet's command menu).

SR: EQUIPMENT CONTENTS SECTION

The last section of the stream report, presents information about material found as equipment contents at the beginning of the batch, during the progress of the batch and at the end of the batch.

12.4 COSTING AND ECONOMIC EVALUATION REPORTS

The following costing and economic evaluation reports can be generated:

- Economic Evaluation Report (EER)
- Cash Flow Analysis Report (CFR)
- Itemized Cost Report (ICR)

12.4a Economic Evaluation Report (EER)

This report includes an executive summary that contains the key results of economic analysis for a project, a listing of all major capital cost items, process summaries for the major components of the operating costs, and finally a comprehensive table with profitability analysis. To generate this report, select menu **Reports ▸ Economic Evaluation (EER)**.

The EER includes the following sections:

1. Executive Summary
2. Major Equipment Specification and FOB Cost
3. Direct Fixed Capital Cost (DFC) Summary
4. Labor Cost - Process Summary
5. Materials Cost - Process Summary
6. Various Consumables Cost - Process Summary
7. Waste Treatment/Disposal Cost - Process Summary
8. Utilities Cost - Process Summary
9. Anual Operating Cost - Process Summary
10. Profitability Analysis

Any one of the above sections may be excluded from the report, if so desired. The options related to the contents of the report are edited from Report Options Dialog: Economic Evaluation Tab.

EER: EXECUTIVE SUMMARY

Most of the key economic indices are contained in this section (see below). The same amount of information is also presented by the interface on the Executive Summary Dialog: Summary Tab (select **View ▸ Executive Summary** from the main menu to view the dialog). The key indices included in the executive summary are:

- **Total Capital Investment**: the total capital cost for the entire process (see 9.2 Total Capital Investment).
- **Capital Investment Charged to This Project**: the fraction of total capital investment that is considered in this economic analysis; this may be less than 100% when the process simulated in this file is part of a multi-product facility (see 9.2f Capital Investment Charged to This Project).
- **Operating Cost**: the annual operating cost (see 9.3 Operating Cost).
- **Credits**: proceeds from streams and/or generated power types denoted as credit; proceeds denoted as ‘credit’ reduce the annual operating cost (see Net Operating Cost below) whereas proceeds denoted as ‘revenues’ increase the total revenues of the project (see Revenues below), see 9.4b Credits. If the annual credits are zero this entry is omitted from this section.
- **Net Operating Cost**: the annual operating cost reduced by the amount of annual credits (see 9.3p Net Annual Operating Cost). If the annual credits are zero this entry is omitted from this section.

- **Revenues**: the total annual revenues (proceeds from streams and generated power types denoted as revenue) of the project; for more details, see 9.4a Revenues.
- **Cost Basis Annual Rate** (aka **Unit Reference Rate**) the flow basis (total flow or component flow) used to convert the annual operating cost to unit production cost (see below). It is also used to convert other annual cost items from an annual basis to a per-unit-reference basis. The main revenue rate is typically used (if defined, see 9.3q Main Product/Revenue Rate) but a special rate can also be provided at the Rate Reference Flows Dialog: Unit Reference tab.
- **Unit Production/Processing Cost**: a per-unit-of-reference operating cost that is calculated by dividing the annual operating cost by the unit reference rate (see 9.3r Unit Reference Rate (or Flow)); for more details, see 9.3n Unit Production/Processing Cost.
- **Unit Production/Processing Revenue**: a per-unit-of-reference revenue term that is calculated by dividing the annual revenues by the unit reference rate (see 9.3r Unit Reference Rate (or Flow)); for more details, see 9.4a Revenues.
- **Gross Margin**: it is a measure of profit that reflects the percentage of annual revenues that become gross profit; for more details, see 9.5a Profitability Analysis.
- **Return On Investment (ROI)**: a profitability measure for the project that can be used to compare different investment options; for more details, see 9.5a Profitability Analysis.
- **Payback Time**: another profitability measure of the project. It represents the time needed for the total capital investment to be recovered by the cumulative net profits; for more details, see 9.5a Profitability Analysis.
- **NPV (at low interest rate)**: yet one more profitability measure (similar to ROI) used to evaluate the viability of an investment or to compare the profitability of a number of different investments. NPV represents the total value of future net cash flows (spread over the lifetime of a project), at the beginning of the project. All future cash flows are discounted to reflect the time-value of money using the lowest of the two interest rates provided at the Economic Evaluation Parameters Dialog: Time Valuation Tab. For more details see 9.5b Cash Flow Analysis.
- **IRR (After Taxes)**: represents the interest rate for which the NPV of a project is zero; can be used as a reference rate to compare with interest rates (after risk assessment is included); for more details, see 9.5b Cash Flow Analysis.

EER: MAJOR EQUIPMENT SPECIFICATION AND FOB COST

This section presents information related to the calculation of the free-on-board (FOB) cost for all equipment resources of the process. More specifically, it includes the following information for each equipment resource:

- **Quantity**: the number of equipment units represented by the equipment resource that are operated in parallel.
- **Standby**: the number of equipment units represented by the equipment resource that correspond to standby units.
- **Staggered**: the number of equipment units represented by the equipment resource that are operated in staggered mode.

- **Description**: this includes a short description of the type and size of the equipment resource.
- **Unit Cost**: this is the FOB cost per equipment unit.
- **Cost**: this is the FOB cost which is calculated by multiplying the unit cost by the total number of equipment units represented by the equipment resource.
- **TOTAL**: this is the total FOB cost of all equipment of the process.

For more details on the above variables, see 9.2a Direct Fixed Capital (DFC).

EER: DIRECT FIXED CAPITAL ESTIMATE SUMMARY

A detailed cost breakdown of the direct fixed capital (DFC) for the entire process. For information on the cost elements appearing in this table, see 9.2a Direct Fixed Capital (DFC).

EER: LABOR COST - PROCESS SUMMARY

It includes the unit cost, annual amount, and annual cost of all labor types that are engaged in the process; for more details, see 9.3c Labor-Dependent Cost.

EER: MATERIALS COST - PROCESS SUMMARY

It includes the unit cost, annual amount, and annual cost of all raw materials utilized in the process; for more details, see 9.3a Materials Cost.

EER: VARIOUS CONSUMABLES COST - PROCESS SUMMARY

It includes the unit cost, annual amount, and annual cost of all consumables utilized in a process; for more details, see 9.3b Consumables Cost.

EER: WASTE TREATMENT / DISPOSAL COST - PROCESS SUMMARY

It includes the unit cost, annual amount and annual cost for treatment/disposal of all material exiting the process and designated as waste (see 6.5b Exiting Material Classification); for more details, see 9.3e Waste Treatment/Disposal Cost.

EER: UTILITIES COST - PROCESS SUMMARY

This section lists the annual amount and cost of all heat transfer agents and power types (collectively referred to as ‘utilities’) involved in the process; for more details, see 9.3d Utilities Cost.

EER: ANNUAL OPERATING COST - PROCESS SUMMARY

This section provides a detailed cost breakdown of the annual operating cost (AOC) for the entire process. For information on the cost elements appearing in this table, see 9.3 Operating Cost.

EER: PROFITABILITY ANALYSIS

This section lists the main figures (capital cost, operating cost, revenues/credits and profits) used by the profitability analysis as well as the main profitability indices (return on investment, payback time, etc.), calculated for the project. Note that this section is only available if the revenues of the project are not zero.

Capital Cost Items:

- **Direct Fixed Capital**: he fixed assets of the investment (for the entire process), such as plant and equipment; for more details, see 9.2a Direct Fixed Capital (DFC).
- **Working Capital**: funds tied-up as required to be available when operating the process; for more details, see 9.2b Working Capital.
- **Startup Cost**: before process becomes operative, any one-time expenditures incurred to prepare the process for operation; for more details, see 9.2c Startup and Validation Cost.
- **Up-Front R&D**: cost of research & development (R&D) required before a product is manufactured (in a new plant); for more details, see 9.2d Up-Front R&D Cost.
- **Up-Front Royalties**: payments for the use of assets, resources, patents, etc. prior to having the whole process in operation; for more details, see 9.2e Up-Front Royalties.
- **Total Investment**: the total capital investment is the sum of the above capital cost elements; for more details, see 9.2 Total Capital Investment.
- **Investment Charged to This Project**: the fraction of the total investment (above) that may be charged to this project may be less than 100% in situations where the process is part of a multi-product facility; for more details, see 9.2f Capital Investment Charged to This Project.

Revenue / Credit Items

For details on the terms in this section, see 9.4 Income.

- **Revenue/Credit Rates**: this part of the table lists the mass flow rates of all streams that are specified as being ‘revenue’ or ‘credit’ streams in a process. A distinction is made between the revenue stream that is specified as the ‘main revenue’ stream through the ‘Stream Classification’ dialog and other revenue streams.
- **Selling/Processing Price for Revenue/Credit**: this part of the table lists the unit prices (selling price or processing fee) of all streams that are specified as being ‘revenue’ or ‘credit’ streams in a process. A distinction is made between the revenue stream that is specified as the ‘main revenue’ stream through the ‘Stream Classification’ dialog and other revenue streams.
- **Revenues/Credits**: this part of the table lists the annual revenues (the product of revenue rates and selling prices) for all streams that are specified as being ‘revenue’ or ‘credit’ streams in a process. A distinction is made between the revenue stream that is specified as the ‘main revenue’ stream through the ‘Stream Classification’ dialog and other revenue streams.
- **Total Revenues**: this corresponds to the total annual revenues of a project.
- **Total Credits**: this corresponds to the total annual credits of a project.
- **Unit Production/Processing Revenue**: this is a reference revenue that is calculated by dividing the annual revenues by the selected flow basis (total flow or component flow) of the stream that is specified as the Unit Reference’ stream through the ‘Rate Reference Flows’ dialog. Depending on whether the selected stream is a process input or output stream, the corresponding unit revenue is denoted as ‘processing’ or ‘production’, respectively; for more details, see 9.4a Revenues.

Operating Cost Items

- **Annual Operating Cost (AOC)**: this is the sum of all operating costs of a plant (represented by the entire process) per year; for more details, see 9.3 Operating Cost.
- **Net AOC**: this is calculated by subtracting the total credits from the actual AOC. Note that this is only displayed when the total credits are not zero.
- **Unit Production/Processing Cost**: this is a reference cost that is calculated by dividing the annual operating cost by the selected flow basis (total flow or component flow) of the stream that is specified as the Unit Reference' stream through the 'Rate Reference Flows' dialog. Depending on whether the selected stream is a process input or output stream, the corresponding unit cost is denoted as 'processing' or 'production', respectively; for more details, see 9.3n Unit Production/Processing Cost.
- **Net Unit Production/Processing Cost**: this is calculated similarly to the unit production/processing cost except that the net AOC is used instead of the actual AOC.

Profitability Analysis Results (Indices)

For details on the terms in this section, see 9.5a Profitability Analysis.

- **Gross Profit**: this is the annual gross profit calculated by subtracting the AOC from the total revenues.
- **Taxes**: this is the fraction of annual gross profit that corresponds to the annual income taxes.
- **Net Profit**: this is the annual net profit calculated by subtracting the annual income taxes from the sum of the annual gross profit and annual depreciable amount; optionally, the latter amount may be excluded from the calculation of the net profit.
- **Gross Margin**: this is a measure of profit that directly tells you what percentage of the annual revenues is gross profit.
- **Return On Investment**: this is another profitability measure used to evaluate the viability of an investment or to compare the profitability of a number of different investments.
- **Payback Time**: this is the time (in years) needed for the total capital investment charged to this project to be exactly balanced by the cumulative annual net profits made over that time.

12.4b Cash Flow Analysis Report (CFR)

This report includes loan information and breakdowns of capital outlay, loan payment and cash flow for each year over the expected lifetime of a project. To generate this report, select menu **Reports ▸ Cash Flow Analysis (CFR)**.

The CFR consists of the following sections:

1. Cash Flow Analysis
2. Loan Information
3. Breakdown of Capital Outlay
4. Breakdown of Loan Payment

Any one of the above sections may be excluded from the report, if so desired. The options related to the contents of the report are edited from Report Options Dialog: Cash Flow Analysis Tab.

CFR: CASH FLOW ANALYSIS

This section presents a cash flow breakdown for each year that the plant for this process is expected to be in operation (see 9.5b Cash Flow Analysis). The calculated net present value (NPV) and internal rate of return (IRR) before and after taxes are also included. More specifically, the following economic variables are included:

- **Capital Investment**: the capital expenses for each year according to the capital outlay of the project. Note that the time schedule used to describe the DFC outlay can span up to five years. The positive capital expenditure in the final year of the project is due to the salvage value of equipment and the recovery of the working capital.
- **Debt Finance**: it represents the amount of money borrowed each year according to the capital outlay of the project.
- **Sales Revenues**: the total revenues for each year according to the operating capacity profile of the project.
- **Operating Cost**: the sum of all operating costs for each year.
- **Gross Profit**: the difference between sales revenues and operating cost for each year.
- **Loan Payments**: it is the fraction of total debt owed that is paid back each year.
- **Depreciation**: it represents the depreciable amount of a project's assets for each year; it can be estimated either based on the straight-line method, or the declining balance method, or sum-of-the-years-digit method (see 9.3o Depreciation).
- **Taxable Income**: the difference between gross profit and loan payments for each year.
- **Taxes**: a percentage on the gross profit that is taken as income taxes for each year.
- **Net Profit**: the sum of gross profit and depreciation minus taxes paid for each year. Note that depreciation may optionally be excluded from the calculation of the net profit (see Economic Evaluation Parameters Dialog: Financing Tab).
- **Net Cash Flow**: the sum of debt finance, net profit and depreciation, minus capital expenses for each year.
- **NPV**: the net present value (NPV) is a profitability measure used to evaluate the viability of an investment or to compare the profitability of a number of different investments; since it factors in the time-value of money it requires an assumed interest rate; it is calculated for three specified interest rates (low, medium and high).
- **Interest %**: three estimates of interest rates (low, medium and high) used to calculate the NPV of the project.
- **IRR After Taxes**: the internal rate of return (IRR) is the interest rate for which the NPV is zero; here, the NPV is calculated based on the net cash flow for each year.
- **IRR Before Taxes**: the interest rate for which the NPV, calculated based on the net cash flow plus income taxes for each year, is zero.

- **Depreciation Method**: the method used to estimate the annual depreciable amount of the project's assets.

CFR: LOAN INFORMATION

This section contains information about the loans taken to finance part of the total capital investment charged to this project. These may include loans for financing the direct fixed capital, working capital, up-front R&D and up-front royalties of a project; for more details on these capital cost items, see 9.2 Total Capital Investment. The following information is listed for each of the above capital cost elements:

- **Amount:** the total amount that needs to be spent for the project.
- **Equity (%):** the percentage of the total amount that comes from equity financing.
- **Debt (%):** the percentage of the total amount that comes from a loan.
- **Interest (%):** the interest rate of the corresponding loan.
- **Loan Time (yrs):** the payment period of the corresponding loan.

For more details on the above variables, see 9.5b Cash Flow Analysis.

CFR: BREAKDOWN OF CAPITAL OUTLAY

This section presents an analysis of how investment capital is distributed among different types of capital expenses over the years throughout the expected lifetime of a project according to its capital outlay. Capital expenses include the direct fixed capital (DFC), working capital, startup cost, up-front R&D and up-front royalties; for more details on capital expenses, see 9.2 Total Capital Investment; for more details on capital outlay, see 9.5b Cash Flow Analysis.

CFR: BREAKDOWN OF LOAN PAYMENT

This section presents an analysis of how loan payments are distributed among different loans and years throughout the expected lifetime of a project according to its capital outlay and loan information. The different loans include those financing the direct fixed capital, working capital, up-front R&D and up-front royalties; for more details on these cost items, see 9.2 Total Capital Investment; for more details on capital outlay and loan payment, see 9.5b Cash Flow Analysis.

12.4c Itemized Cost Report (ICR)

This report presents the various cost components of the total annual operating cost (AOC):

1. Cost of Materials
2. Labor-Dependent Cost
3. Facility-Dependent Cost
4. Cost of Consumables
5. Laboratory, Quality Control (QC), Quality Analysis (QA) Cost
6. Waste Treatment and Disposal Cost
7. Utilities Cost
8. Cost of Transportation

9. Miscellaneous (advertising, selling cost, royalties, etc.)

You may exclude some of the components that contribute to the total AOC of a process through the Operating Cost Options Dialog. To access this dialog, select menu item **Edit ▸ Process Options ▸ Operating Cost Options** from the main menu (or select **Operating Cost Options** from the flowsheet's command menu).

To generate the itemized cost report, select menu **Reports ▸ Itemized Cost (ICR)**. The default options for the generation of this report can be modified through the Report Options Dialog: Itemized Cost Tab. To access this dialog, select menu **Reports ▸ Options** from the main menu of the application.

The running cost and its components are accumulated on a per year basis but they can be reported in this report on either per year (default) or per batch (for batch processes) or per unit of reference rate (see 9.3r Unit Reference Rate (or Flow)).

By default, no charts are included in the ICR (e.g. pie charts showing the various components of the AOC). To include charts, make sure you check the 'Include Charts' option in Report Options Dialog: Itemized Cost Tab.

The ICR includes the following sections:

1. Overall Process Parameters
2. Cost Per Process Section
3. Breakdown per Cost Item and per Section
4. Material Cost
5. Labor Cost
6. Consumables Cost
7. Waste Treatment / Disposal Cost
8. Utilities Cost

ICR: OVERALL PROCESS PARAMETERS

This section lists the key production parameters of the process. These include the following:

- **Operating Time**: the assumed annual operating time for the process.
- **Annual Production/Processing Rate**: the reference rate (on a per stream or per component-in-a-stream basis) that was used to convert the annual operating cost to per-unit-of-reference cost. The application uses the Main Product/Revenue Rate Stream (as defined in the Stream Classification Dialog) as unit reference rate for this report but if needed, users can select another definition for the Unit Reference Rate' based on any process stream using the Rate Reference Flows Dialog: Unit Reference tab. Depending on whether the unit reference rate used is based on a process input or output stream, the corresponding rate is denoted as 'processing rate' (if it is based on an input stream) or 'production rate' (if it is based on an output stream).
- **Recipe Batch Time**: the time required to complete a single batch.
- **Recipe Cycle Time**: the time between the start of two consecutive batches.
- **Number of Batches per Year**: the number of batches processed in a calendar year.

ICR: COST PER PROCESS SECTION

Assuming that the AOC of the process is the sum of AOC contributions of each process section, this part of the report shows how the each process section's AOC contribution breaks down to all of the components that make up the operating cost (materials, labor, facility-dependent, etc.). Each cost item is expressed per reference amount, per batch and per year.

The sum of AOC over all process sections may be lower than the AOC of the entire process as it does not account for the miscellaneous cost component (advertising/selling costs, running royalties and failed product disposal cost). This cost is only calculated at the process level and it cannot be associated with any particular section of the process.

ICR: BREAKDOWN PER COST ITEM AND SECTION

Assuming that the AOC of the process is the sum of all of the AOC's cost items (materials, labor, etc.) this part of the report shows how each of the component cost items distribute to each of the process sections. Remember that a user may exclude (if need be) any of the component items (see Operating Cost Options Dialog). The costs are presented only at the cost basis chosen for the report (per year, per batch or per-unit-reference). If charts are included, this information may also be presented in the form of a pie chart.

ICR: MATERIAL COST

Since material cost can be the biggest contributor to the total AOC of a process, this section presents various cost breakdowns of the material cost component of the AOC in order for the user to better understand where are the 'hot spots' for material cost. The three most important origins for material consumption are: as raw materials, as cleaning agents and as heat transfer agents. If requested, the consumption of each material on a per-origin basis can also be included. The total material cost and the costs per material consumption origin are presented in four corresponding subsections. These are:

1. Material Cost
2. Raw Material Cost
3. Cleaning Agent Cost
4. Heat Transfer Agent Cost

By default, only the first subsection is included in the ICR. For each subsection, four different cost breakdowns of increasing level of detail are presented in lower-level subsections:

(a) Section Summary

(b) Breakdown by Section

(c) Breakdown by Material Type

(d) Detailed Breakdown by Material Type

Similar lower-level subsections are included in the remaining three subsections. The contents of each lower-level subsection are explained below:

- **Section Summary**: This includes a cost breakdown by process section. The costs are presented in the selected cost basis (per year, per batch, or per reference amount). Optionally, this information may also be presented in the form of a chart.

- **Breakdown by Section**: This includes a cost breakdown by process section and then by material type. For each process section, the unit cost, amount and total cost of each material type utilized in that section is presented. The latter two costs are presented in the specified cost basis (per year, per batch, or per reference amount).
- **Breakdown by Material Type**: This includes a cost breakdown by material type and then by process section. For each material type, the unit cost, amount and total cost of that material type are listed for every section that uses it. The latter two costs are presented in the specified cost basis (per year, per batch, or per reference amount).
- **Detailed Breakdown by Material Type**: This includes a cost breakdown by material type, then by process section, and then by procedure. For each material type and for each section, the unit cost, amount and total cost of that material type are listed for every procedure of that section that uses it. The latter two values are presented in the specified cost basis (per year, per batch, or per reference amount).

If a process contains many unit procedures, the detailed breakdown per material type can become very long resulting in an exceeding long ICR. This portion of the ICR may be of interest for users who do not use process sections to breakdown their process representation.

For more details on the variables listed in this section, see 9.3a Materials Cost.

ICR: LABOR COST

This section presents various cost breakdowns of a project's labor cost. Four different cost breakdowns of increasing level of detail are presented in the following subsections:

1. Section Summary
2. Breakdown by Section
3. Breakdown by Labor Type
4. Detailed Breakdown by Labor Type

The contents of each subsection are explained below:

- **Section Summary**: This includes a cost breakdown by process section. The costs are presented in the specified cost basis (per year, per batch, or per reference amount). Optionally, this information may also be presented in the form of a chart.
- **Breakdown by Section**: This includes a cost breakdown by process section and then by labor type. For each process section, the unit cost, amount and total cost of each labor type utilized in that section is presented. The latter two costs are presented in the specified cost basis (per year, per batch, or per reference amount).
- **Breakdown by Labor Type**: This includes the following two tables:
  - **(a)** a summary table that lists the adjusted basic rate, lumped basic rate, annual amount and total cost of all labor types that are currently in use by the process; the total cost is presented in the specified cost basis (per year, per batch, or per reference amount);
  - **(b)** a cost breakdown by labor type and then by process section; for each labor type, the unit cost, amount and total cost of that labor type are listed for every section that uses it. The

latter two values are presented in the specified cost basis (per year, per batch, or per reference amount).

- **Detailed Breakdown by Labor Type**: This includes a cost breakdown by labor type, then by process section, and then by procedure. For each labor type and for each section, the unit cost, amount and total cost of that labor type are listed for every procedure of that section that uses it. The latter two values are presented in the specified cost basis (per year, per batch, or per reference amount).

For more details on the variables listed in this section, see 9.3c Labor-Dependent Cost.

ICR: CONSUMABLES COST

This section presents various cost breakdowns of the process consumables cost. Four different cost breakdowns of increasing level of detail are presented in the following subsections:

1. Section Summary
2. Breakdown by Section
3. Breakdown by Consumable Type
4. Detailed Breakdown by Type

The contents of each subsection are explained below:

- **Section Summary**: This includes a cost breakdown by process section. The costs are presented in the specified cost basis (per year, per batch, or per reference amount). Optionally, this information may also be presented in the form of a chart.
- **Breakdown by Section**: This includes a cost breakdown by process section and then by consumable type. For each process section, the unit cost, amount and total cost of each consumable type utilized in that section is presented. The latter two costs are presented in the specified cost basis (per year, per batch, or per reference amount).
- **Breakdown by Consumables Type**: This includes a cost breakdown by consumable type and then by process section; for each consumable type, the unit cost, amount and total cost of that consumable type are listed for every section that uses it. The latter two values are presented in the specified cost basis (per year, per batch, or per reference amount).
- **Detailed Breakdown by Type**: This includes a cost breakdown by consumable type, then by process section, and then by procedure. For each consumable type and for each section, the unit cost, amount and total cost of that consumable type are listed for every procedure of that section that uses it. The latter two values are presented in the specified cost basis (per year, per batch, or per reference amount).

For more details on the variables listed in this section, see 9.3b Consumables Cost.

ICR: WASTE COST

This section presents various cost breakdowns of the process waste treatment/disposal cost. Four different cost breakdowns of increasing level of detail are presented in the following subsections:

7.1 Section Summary

7.2 Breakdown by Section

7.3 Breakdown by Waste Type

7.4 Detailed Breakdown by Waste Type

The contents of each subsection are explained below:

- **Section Summary**: This includes an amount and cost breakdown by process section. The corresponding values are presented in the specified cost basis (per year, per batch, or per reference amount). Optionally, this information may also be presented in the form of a chart.
- **Breakdown by Section**: This includes a cost breakdown by process section and then by waste type. For each process section, the unit cost, amount and total cost of each waste type of that section is presented. The latter two costs are presented in the specified cost basis (per year, per batch, or per reference amount).
- **Breakdown by Waste Type**: This includes a cost breakdown by waste type and then by process section; for each waste type, the unit cost, amount and total cost of that waste type are listed for every section in which it is present. The latter two values are presented in the specified cost basis (per year, per batch, or per reference amount).
- **Detailed Breakdown by Waste Type**: This includes a cost breakdown by waste type, then by process section, and then by procedure. For each waste type and for each section, the unit cost, amount and total cost of that waste type are listed for every procedure of that section in which it is present. The latter two values are presented in the specified cost basis (per year, per batch, or per reference amount).

For more details on the variables listed in this section, see 9.3e Waste Treatment/Disposal Cost.

ICR: UTILITIES COST

This section presents various cost breakdowns of the process utilities cost. Four different cost breakdowns of increasing level of detail are presented in the following subsections:

1. Section Summary
2. Breakdown by Section
3. Breakdown by Utility Type
4. Detailed Breakdown by Utility Type

The contents of each subsection are explained below:

- **Section Summary**: This includes two tables:

  (a) an amount and cost breakdown of electricity by process section.

  (b) an amount and cost breakdown of heat transfer agents by process section

  The corresponding values are presented in the specified cost basis (per year, per batch, or per reference amount). Optionally, this information may also be presented in the form of a chart.
- **Breakdown by Section**: This includes a cost breakdown by process section and then by utility type. For each process section, the unit cost, amount and total cost of each utility type of that section is presented. The latter two costs are presented in the specified cost basis (per year, per batch, or per reference amount).
- **Breakdown by Utility Type**: This includes a cost breakdown by utility type and then by process section; for each utility type, the unit cost, amount and total cost of that utility type

are listed for every section that uses it. The latter two values are presented in the specified cost basis (per year, per batch, or per reference amount).

- **Detailed Breakdown by Utility Type**: This includes a cost breakdown by utility type, then by process section, and then by procedure. For each utility type and for each section, the unit cost, amount and total cost of that utility type are listed for every procedure of that section that uses it. The latter two values are presented in the specified cost basis (per year, per batch, or per reference amount).

For more details on the variables listed in this section, see 9.3d Utilities Cost.

12.5 THROUGHPUT ANALYSIS REPORT (THR)

SuperPro Designer is equipped with powerful throughput analysis and debottlenecking capabilities. The objective of these features is to allow the user to quickly and easily analyze the capacity and time utilization of each equipment resource and to identify opportunities for increasing throughput with the minimum possible capital investment. An in-depth coverage of the principles behind how throughput analysis and debottlenecking can be done with SuperPro Designer can be found in Chapter 11 (Debottlenecking).

To generate this report, select menu **Reports ▸ Throughput Analysis (THR)** from the main menu of the application.

The thoughput and debottlenecking report can display the following sections:

1. Process Parameters
2. Equipment Capacity
3. Throughput Increase
4. Detailed Throughput Increase

Any of the above sections can be included or omitted from the report. All content customization for this report can be made from the Report Options Dialog: Throughput Analysis Tab. To access this dialog, select menu **Reports ▸ Options** from the main menu of the application

THR: PROCESS PARAMETERS

This section displays information on the annual operating time, the current annual and batch throughput, the number of batches per year, and the time bottleneck equipment.

THR: EQUIPMENT CAPACITY

The next section displays information on Equipment Size/Throughput Utilization, Equipment Uptime, and Combined Utilization for all the procedures of a process. The procedure with the highest Combined Utilization is considered the Throughput (Size) Bottleneck based on this approach. Please note that this may not be the true bottleneck under real world conditions. Equipment items that are in Design Mode do not appear on these tables because their size is calculated by the program to meet the current processing demand.

THR: THROUGHPUT INCREASE

The third section is a summary of potential maximum throughput (PMT) under conservative, realistic and theoretical assumptions for equipment uptime (for the exact definition of the terms used, see Definitions & Theory of Throughput Analysis. It also identifies the bottlenecks (limiting procedure and equipment item) under each assumption. For each category, the bottleneck is the procedure with the lowest value of PMT. The bottleneck identified based on the theoretical PMT approach is always the same as the one identified by the Combined Utilization approach (previous table).

THR: DETAILED THROUGHPUT INCREASE

The rest of the report displays the individual potential throughput figures for each unit procedure, based on the Conservative, Realistic, and Theoretical assumptions. Furthermore, the limiting procedure and equipment bottlenecks are identified for each section of the process in their respective Section Summaries.

12.6 ENVIRONMENTAL REPORTS

There are two reports that present information related to the environmental impact of the process:

- Environmental Impact Report (EIR)
- Emissions Report (EMS)

12.6a Environmental Impact Report (EIR)

This report presents information that describes the effects of the process output streams on the environment. Furthermore, it contains a detailed bookkeeping of all chemicals that are either regulated by the EPA or tagged as hazardous by the user. To generate this report, select menu **Reports ▸ Environmental Impact (EIR)** from the main menu of the application.

The report itself is composed of the following sections:

1. Waste By Type
2. Waste by Section
3. Streams
4. Overall Balance
5. Component Fate
6. Sara 313 Chemicals
7. 33/50 Chemicals
8. Solid Waste
9. Aqueous Waste
10. Organic Waste
11. Emissions Section
12. Hazardous Streams Section

13. Pollution Indices Section

Any of the above sections can be included or omitted from the report. All content customization for this report can be made from the Report Options Dialog: Environmental Impact Tab. To access this dialog, select menu **Reports ▸ Options** from the main menu of the application.

EIR: WASTE BY TYPE

This section lists the amount of each component /mixture classified as waste under the different waste categories (aqueous, organic, solid, emissions). The amounts are expressed in terms of kg/kg of Main Product, kg/yr, kg/batch, and as % of the category waste.

EIR: WASTE BY SECTION

This section lists the amount of each component /mixture classified as waste under the different waste categories (aqueous, organic, solid, emissions) for each process section.

EIR: STREAMS

This section is somewhat similar to the first section of the stream report. Each stream is described by its name, source and destination procedure (or INPUT/OUTPUT). Then the list of its environmental and aqueous properties is included (TOC, COD, ThOD, etc.) as concentrations (in mg/l) and daily demands (kg carbon/day or kg oxygen/day.)

EIR: OVERALL BALANCE

This section presents the total environmental load increase or decrease as reflected by the values of TOC, COD, etc. of all streams entering and leaving the process. It contains two tables: one presents the values either on-a-per-hour-basis (only choice for continuous processes) or on-a-per-batch basis (choice available for batch processes); the second table has the same numbers on a yearly basis. Notice that the second table (yearly values) also reports the percentage reduction (or increase if the value is negative) of each environmental index.

EIR: COMPONENT FATE

It is becoming ever more imperative for managers responsible for the operation of manufacturing and wastewater treatment facilities to be aware of the ultimate destination of each chemical as they leave the plant's battery limits as either solid or liquid waste (organic /aqueous) or gaseous releases to the atmosphere (emissions). This section presents the allocation of each chemical that either enters or is produced by the plant facility to all waste gateways. The first column presents the cumulative amounts of each chemical entering on any of the input streams of the plant, and the next three columns present the amounts leaving the plant on all waste streams (solid, liquid streams and gaseous).

EIR: SARA 313 CHEMICALS

Two groups of chemicals demand special attention for regulatory purposes: one group includes all the chemicals that must be included in the SARA 313 report as required by US government regulations; the other is the group of chemicals required to be present in the 33/50 reduction plan, as dictated by government regulations. This section deals with the first group (and the next section with the other). It presents an accurate account of all SARA 313 chemicals

entering and leaving the plant as well as their difference. It should be mentioned that in order for a component to be included in this section, its 'Is SARA 313' flag must be set to TRUE.

EIR: 33/50 CHEMICALS

Similar to the previous section, only dealing with 33/50 chemicals. In order for a component to be included in this section, its 'Is 33/50' flag must be set to TRUE.

EIR: SOLID WASTE

You can classify the output streams of a process file as Solid Waste, Organic Waste, Aqueous Waste, or Emission. This section deals with the description of all streams classified as Solid Waste. It consists of two parts. The first part enumerates all streams that are characterized as solid waste by listing their composition (weight %), flowrate (in kg/h) and annual flowrate (kg/year). The second part, presents a detailed accounting from the component point of view; it shows how the total amount of each component leaving as solid waste is distributed in each stream. It should be mentioned that you can specify some components not to be listed in this section of the EIR report by setting the component property 'Is Tracked in Solid Waste' to FALSE (all components have this flag set to TRUE by default.).

EIR: AQUEOUS WASTE

Similar to the Solid Waste Section, only deals with streams classified as aqueous (liquid) waste.

EIR: ORGANIC WASTE

Similar to the Aqueous Waste Section, only deals with streams classified as organic (liquid) waste.

EIR: EMISSIONS

Similar to the Solid Waste Section, only deals with streams classified as emissions (gaseous waste). A dedicated report presents much more details on emissions (see 12.6b Emissions Report (EMS)).

EIR: HAZARDOUS STREAMS

Some components can be tagged by the user as hazardous when present in a stream at a concentration higher than a specified threshold. The presence of such components in output streams, automatically tags the streams as hazardous. Furthermore, you may explicitly tag a stream as hazardous yourself, if so desired (see Classification of Input and Output Streams). In this section of the report, the hazardous streams are presented. The format of this section is similar to those of waste streams.

EIR: POLLUTION INDICES

The last section of the EIR report presents certain ratios that are indicative of the environmental kindness (or lack thereof) of a process file. The first index presented applies to processes that have a main revenue stream (e.g. manufacturing facilities with a main product stream). It reports the ratio of total amount of waste (solid, aqueous, organic, and emissions) produced per kg of main revenue stream processed. The next five indices apply to processing plants that employ raw materials. It reports the ratio of total waste, solid waste, aqueous waste, organic waste, and emissions produced per kg of raw material utilized.

12.6b Emissions Report (EMS)

This report presents information on air pollutant amounts from all the procedures of the process. To generate this report, select menu **Reports ▸ Emissions (EMS)**. For more details on Emission Calculations, see Chapter 10 (Emissions).

The IDR consists of the following sections:

1. Overall Process Data
2. Procedure-Averaged Category Rates & Totals (per Procedure)
3. Category Amount Totals (per Batch)
4. Procedure-Averaged Component Rates (per Procedure, per Operation)
5. Operation-Averaged Component Rates (per Procedure, per Operation)
6. Time-Averaged Component Rates (per Component)
7. Component Amount Totals (per Procedure, per Batch)

Any of the above sections may be included or excluded from the report by visiting the customization page at Report Options Dialog: Emissions Tab. To access this dialog, select menu **Reports ▸ Options** from the main menu of the application.

EMS: OVERALL PROCESS DATA

This table displays information about the overall process (Plant Batch time, number of Batches per year for batch processes, and Operating days per year for continuous processes).

EMS: PROCEDURE-AVERAGED CATEGORY RATES & TOTALS (PER PROCEDURE)

This section presents information on air pollutant flow (lumped per pollutant category) from the various procedures of a process. The flowrates (in kg/h) represent average flows during the cycle of a procedure

You should classify all the chemicals that appear in your process file (especially those that can potentially be emitted) into one of the pollutant categories (see 3.3 Pollutant Categorization Guidelines).

For each procedure, the Actual and Permit Allowable flowrates of the following pollutant categories are included:

(a) Total Particulate (and its various subcategories),
(b) Total VOC (and its various subcategories),
(c) Acid Gases (and its two subcategories),
(d) Extremely Toxic Gases (ETG) and its two subcategories,
(e) Carbon Monoxide (CO),
(f) NOx,
(g) SO2 and
(h) Bases

Up to four additional pollutant categories (of your own choosing) with their limits can also be defined see *Emission Limits Dialog*).

You can set emission limits for the various pollutant categories above, except for volatile organic compounds (VOCs) (see Emission Limits Dialog). You can access this interface from the main menu by selecting ***Edit*** ▸ ***Process Options*** ▸ ***Preferences*** ▸ ***Emission Limits*** *or from the flowsheet's context menu by selecting* ***Preferences*** ▸ ***Emission Limits****. For VOCs the emission limit is calculated by the program based on the composition of the various vent (emission) streams. The emissions report will include warnings if the accumulated emissions for any of the above categories exceeds the set limit.*

EMS: CATEGORY AMOUNT TOTALS (PER BATCH)

This section provides the total amounts on a per batch basis for each pollutant category.

The following four tables will provide users with enough information that will pinpoint any emission violating operations and data that can be used in filing required emission reports:

EMS: PROCEDURE-AVERAGED COMPONENT RATES (PER PROCEDURE, PER OPERATION)

This section will include a table for each procedure in the recipe. The rates presented are calculated as the amount of component emitted divided by the procedure's total time. Since all rates have a common time reference (albeit somewhat arbitrary) they can be summed up, so totals per procedure are also presented.

EMS: OPERATION-AVERAGED COMPONENT RATES (PER PROCEDURE, PER OPERATION)

This section will include a table for each procedure in the recipe. Each table will present an operation-averaged emission rate (amount emitted divided by the corresponding operation's process time). Since each rate is calculated on a different time basis, no totals are presented.

EMS: TIME-AVERAGED COMPONENT RATES (PER COMPONENT)

The previous two sections that showed component emission rates failed to realistically capture overlapping effects between operation in the same or different procedures. In other words, if a component is emitted (during the same period) by two different operations the combined amount would not be captured. This section, presents a table for each component emitted. Each table is organized in time intervals (user-selectable, usually 1 hr). For each time-slice, we present all operations that emit that component and the corresponding rate, as well as a cumulative rate representing the combined effect of all operations that happen to be active in that interval. The size of the time-averaging interval and its units can be specified from the interface of the options of this report.

EMS: COMPONENT AMOUNT TOTALS (PER PROCEDURE, PER BATCH)

This section will include a table for each procedure in the recipe. Each table will have as many rows as the operations in that procedure and columns corresponding to (any) components present in any emission streams that are outputs in that operation. Each cell shows the component amount per batch emitted by that operation if it is a batch process or the component amount per day for a continuous process. Totals (per procedure) are also presented.

12.7 EQUIPMENT REPORT (EQR)

This report includes listings (summary and detailed descriptions) for all main and auxiliary equipment resources involved in the process as well as any consumables that may be used by the equipment. To generate this report, select menu **Reports ▸ Equipment (EQR)**.

The EQR consists of the following sections:

1. Equipment Summary
2. Itemized Equipment List
3. CIP Skid List
4. SIP Panel List
5. Consumables

Any one of the above sections may be excluded from the report, if so desired. The options related to the contents of the report are edited from Report Options Dialog: Equipment Tab.

EQR: EQUIPMENT SUMMARY

Presents a list of all equipment resources used in the process along with their size (per unit), purchase cost (per unit), and material of construction. For each equipment resource, the number of units used simultaneously, in a staggered set or requested as stand-by is also reported.

EQR: ITEMIZED EQUIPMENT LIST

Contains as many paragraphs as equipment resources in the process. For each equipment, a list of attributes is presented. The first few attributes are common to all equipment types (e.g. size mode, number of units, number of standby units, etc.) while the rest depend on the equipment type.

EQR: CIP SKID LIST

Lists all CIP (cleaning-in-place) skids, the equipment, procedure and operation that use each skid, and their scheduling summary. As CIP skids may be of great importance (esp. in multi-product facilities) a dedicated report presents more detailed information (incl. sizing, see 12.8 CIP & SIP Report (CSR)).

EQR: SIP PANEL LIST

Lists all SIP (steam-in-place) panels, the equipment, procedure and operation that use each panel, and their scheduling summary.

EQR: CONSUMABLES

A list of any consumables (required or optional) that may be used by equipment in the process. Consumables are assigned to equipment from their Equipment Data Dialog: Consumables Tab.

12.8 CIP & SIP REPORT (CSR)

This report contains information on the sizing of CIP skids and steam usage by SIP panels. It presents a table for each CIP skid utilized in the process with a list of the cleaning steps that are considered for sizing that skid. The tables within the CIP & SIP Report also include the cleaning volume, flowrate, duration and recirculation times. Other tables include the volume of each cleaning agent that is consumed by CIP operations as well as through non-CIP operations whose input streams are classified as "Cleaning Agent" through the Stream Classification Dialog. Additional tables provide information on the type and amount of utilities consumed during SIP operations. To generate this report, select menu **Reports ▸ CIP & SIP (CSR)**.

You can customize the appearance of this report from Report Options Dialog: CIP & SIP Tab.

To associate a CIP skid with a given operation and include that operation in the sizing calculation provided by this report, the "Consider in Skid Sizing?" checkbox must be checked on within the

12.9 INPUT DATA REPORT (IDR)

This report contains all the input information either provided or accepted by the user and therefore used to execute the mass & energy balances and perform the economic evaluation. It can be very useful for documenting a process file, or for attempting to identify sources of error that lead to unexpected simulation results. Since the process file is saved in a proprietary format (not readable by anything else other than the program itself), engineers and scientists could use the IDR report as an alternative way to communicate the exact specifications of a process created by the program. To generate this report, select menu **Reports ▸ Input Data (IDR)**.

The IDR consists of the following sections:

1. Registered Components & Their Properties
2. Preferences
3. Input Stream Data
4. Procedure and Operation Data
5. Process Scheduling Data
6. Equipment & Labor Data
7. Economic Data

Any one of the above sections may be excluded from the report, if so desired. The options related to the contents of the report are edited from Report Options Dialog: Input Data Tab.

IDR: REGISTERED COMPONENTS & THEIR PROPERTIES

Contains all the components and their property values as set in the current process file; it also contains the components designated as biomass, water and activity assessment. It also reports which component properties have been used during the last run of the simulation.

PREFERENCES

Contains information on the stream report format.

INPUT STREAM DATA

Contains the description of each process input stream (name, temperature, pressure and component composition).

IDR: PROCEDURE & OPERATION DATA

Lists all procedures and related data. For each procedure a detailed listing of the operations included is also mentioned along with all the operation-specific information (other than scheduling-related data that is mentioned later in this report) that were either typed in by the user or were assigned defaults by the program and accepted by the user.

IDR: PROCESS SCHEDULING DATA

Includes the scheduling data set for the whole process (annual operating time, either number of batches or batch efficiency) and the scheduling data for each operation (setup time, process time, turnaround time, start time shift).

IDR: EQUIPMENT AND LABOR PARAMETERS

Contains an equipment related table with several equipment related parameters such as the number of standby units, the material of construction, the material factor, the installation factor, the maintenance factor for labor and the maintenance factor for materials. Also contains a labor related table with one entry for each operation for each operation (with the batch labor factor, the continuous labor factor, the maintenance factor for labor and the maintenance factor for materials.

IDR: ECONOMIC DATA

Contains tables with:

(a) **Cost Multipliers**
All cost multipliers used to estimate the total investment (piping, instrumentation, insulation, electrical work, etc.), the total operating cost (fringe benefits, supervision, laboratory etc.) and the labor requirements (warehouse, packaging, etc.) Also contains multipliers for Fixed Capital Cost Estimation.

(b) **Main Product Rate Stream and By-products**
Contains the stream designated as the main product rate stream (if any) and the any other streams designated as secondary sources of revenue (by-products). For each such stream, its rate and the revenue per unit produced (or processed) is also reported.

(c) **Raw Materials**
Contains a listing of all streams designated as raw materials along with their purchase prices.

(d) **Waste Treatment and Disposal Cost**
Contains a listing of all streams designated as waste (solid, liquid or emissions), along with their required waste treatment costs per unit of waste.

12.10 CUSTOM EXCEL REPORT

This report has fully customizable content that is formatted as a multiple worksheet Excel book. Before you create the report, you must visit the Report Options Dialog: Custom Excel Tab in order to specify what information you wish to have included in the report (select **Reports ▸ Options** from the main menu, and then visit the 'Custom XL' tab). The content of the report is organized in sections and each section contains one or more sub-sections.The sub-sections may also contain multiple items that may be included/excluded. Each section included in the report will end up as a separate worksheet in the 'xls' file. The sections which may be included are:

1. General
2. Materials
3. Utilities
4. Stream Summary
5. Unit Procedures
6. Equipment
7. Scheduling
8. Wastes
9. Consumables
10. Storage Units
11. Labor

Some sections may contain as little as one sub-section with one item; others may contain several sub-sections with multiple items within each sub-section. Some sub-sections allow you to include tables (e.g. stream summary table, or equipment contents) or charts (e.g. operations gantt chart, or a selected material's resource consumption or inventory chart).

XLR: GENERAL SECTION (WORKSHEET)

This section may include any of the following sub-sections:

- **Description**: this can contain any information related to the process as a whole: the process flowsheet, the name of the file, the name of the engineer responsible for the project, the name of the project, etc.
- **Size:** this reports the process throughput (batch size) and/or the annual throughput.
- **Scheduling** (available for batch processes only): this can include scheduling information such as the process batch time, cycle time, number of batches per year, bottleneck equipment, etc. More-detailed scheduling information can also be included as a separate worksheet (as part of the 'Scheduling' section (see below).
- **Economics**: any key economic figures of the process: total capital investments, total revenues, operating cost etc.

- **Project Indices**: indices resulting from the economic evaluation of the project (gross margin, return on investment, payback time, IRR before & after tax etc.)

XLR: MATERIALS SECTION (WORKSHEET)

This section may include any of the following sub-sections:

- **Tables:** this may include tables presenting the consumption, output, or cost of selected material(s) as well as the overall material balances.
- **Charts**: this includes pure component or stock mixture consumption tracking charts, material output charts, and inventory charts.

XLR: UTILITIES SECTION (WORKSHEET)

This section may include any of the following sub-sections:

- **Tables:** items in this sub-section include demand tables for all power types or heat transfer agents, as well as the cost tables of these resources. Tables for utility loads associated with each individual operation may also be generated.
- **Charts**: items in this sub-section include consumption and/or inventory charts for heat transfer agents, and power demand /generation charts for a selected power type.

XLR: STREAM SUMMARY SECTION (WORKSHEET)

This section contains only one sub-section with one item: the stream summary table of the process.

XLR: UNIT PROCEDURES SECTION

This section includes sub-sections that each map to a selected procedure in the process. For each of the selected procedure(s), the Activity Overview Table (which describes the list of activities carried out by the operations in the procedure's queue) is included.

XLR: EQUIPMENT SECTION

This section may include any of the following sub-sections:

- **Tables:** This can include a summary listing of all equipment resources included in the process, as well as the equipment contents of a selected equipment resource.
- **Charts**: two possible items may be included here: the equipment occupancy chart for the process and the throughput analysis charts (Utilization factors and Throughput potential).

XLR: SCHEDULING SECTION

This section may include the following sub-sections:

- **Key Scheduling Variables**: this includes the process batch time, cycle time, number of batches per year, minimum cycle time, maximum number of batches per year, available & utilized annual operating time, the longest procedure, and the bottleneck equipment.

- **Charts:** this can include the equipment occupancy chart and/or the operation/equipment gantt charts.

XLR: WASTES SECTION

This section includes only one sub-section: the **Waste Generation Tables**. There may be up to five items included in this sub-section: up to four tables dedicated to each of the four distinct waste types allowed by the application (solid, aqueous, organic and emissions), and a fifth table presenting all waste cumulatively.

XLR: CONSUMABLES

This section includes a table with all the consumables used in the process. The table shows consumable demand amounts and cost.

XLR: STORAGE UNITS

This section can include charts of supply unit material demand and receiving unit material deposit as well as the inventory charts for the material storage units.

XLR: LABOR SECTION (WORKSHEET)

This section may include any of the following sub-sections:

- **Tables:** items in this sub-section may include a demand table for all labor types, as well as the cost table of all the labor type resources.
- **Charts**: this includes consumption charts for each selected labor type associated with the selected Unit Procedures chosen in the Unit Procedures section of this dialog.

12.11 GENERATE-AND-SAVE A REPORT SET

Every time you choose a **Reports ▸ <Report-Type>** command from the application's main menu, a new report file is created and saved in the same folder as the process file under the same name. The exact name depends on the name of the process file and the type of the report: for example, for a process file named "ProjectX.spf" the file created to contain the materials and streams report (SR) is: "ProjectX_SR"; the file's extension depends on the preferred format for the report; if a 'pdf' (Adobe) format was the choice, then the extension would be ".pdf" thus the full name for the report file would be "ProjectX_SR.pdf". Since the same file name (and location) is always selected to execute a given report generation (and view) command, if a previous version of the report was created previously, the new command will overwrite the pre-existing file in favor of creating the new one. Sometimes, it is desired to keep one (or more) reports and save them away as they may represent some distinct state of the process. Perhaps some key operating parameters were assigned a set of values, and before you change them and re-create the reports, you may wish to keep one (or more) reports saved away to compare with future reports when the key parameters of the process assume new values. One way of accomplishing this task (preferred) is to save the state of the process in a separate file, then generate the reports. Since the name of the report files depend on the saved name of the process files, the new reports will be distinct from previously generated reports. If for some reason, you

do not wish to save the process file under a special name, then you can simply create the desired reports and have them kept in a safe location by selecting **Reports ▸ Create & Save As** from the main option of the application. The Create and Save Multiple Reports Dialog will appear. From that dialog you may specify:

1. The report(s) that you wish to have the application create.
2. A set of names (one for each created report) and a folder where you wish to keep the report files. The application by default will suggest the automatic names generated for each report. If you were to accept those names, then a folder other than the process file's folder should be selected.

After you exit the dialog with OK, the application will create all the requested report files and saved them under the designated folder.

You can either use the default subtitle or specify your own subtitle. The default subtitle ("for <FileName>") will automatically copy the filename of the project file into the reports. This default subtitle could be modified to include additional information, such as "Final Results for the <FileName> process, as verified by John Smith". If the filename in this scenario was BetaGalactosidase, the first page of each report would include the statement "Final Results for the BetaGalactosidase process, as verified by John Smith".

13 VISUAL OBJECTS

In order to represent the mass and material transformations in a process, we need only two types of objects: unit procedures and streams. Elsewhere you can find extensive descriptions of the visual as well as the functional properties of each of these elements (see Streams and Procedures & Operations). However, oftentimes, the drawing of a flowsheet can be enhanced by including several other non-functional elements (i.e., elements without any modeling behind them). For instance, you may need to border a certain section of the process by a bounding rectangle and assign it a name, since it represents a particular sub-section of the entire plant (e.g., the raw materials pre-treatment section, or the x-chemical removal section, etc.). In other cases, the designer of a particular process, may wish to comment on certain steps, so she/he may want to place some text right under a particular step. All these new elements that can be added to enhance the visual appearance of a process flowsheet but have no effect on the physico-chemical transformations occurring in it, we will call Visual Objects.

Information on the Visual Objects is organized in the following topics:

- Types of Visual Objects
- Adding a New Visual Object
- Editing Existing Visual Objects
- Visual Objects Toolbar
- Editing the Style of Visual Objects

13.1 TYPES OF VISUAL OBJECTS

SuperPro Designer supports the following types of visual objects:

- Lines
- Polylines
- Rectangles / Squares
- Round Edge Rectangles / Round Edge Squares
- Ellipses / Circles
- Polygons
- Text

All visual objects can be inserted in a flowsheet by using the Visual Objects toolbar. The toolbar can be visible or hidden. Obviously, when you work on the engineering aspects of a process file, you don't want your work area to be cluttered so the palette is originally invisible.

To show or hide the Visual Objects toolbar, click **Toggle Visual Objects Toolbar** ( ) on the **Main** toolbar, or select **Visual Objects Toolbar** on the **View** menu, or right-click on any toolbar and select **Visual Objects** on the shortcut menu that appears. For more information on this toolbar, see 13.5 Visual Objects Toolbar.

13.2 ADDING A NEW VISUAL OBJECT

In order to insert a new visual object, the Visual Objects Toolbar must be showing. Please see 13.1 Types of Visual Objects for information on how to show or hide this toolbar. To insert one of the seven types of visual objects available, you will use the first eight (8) buttons of the toolbar displayed in four rows. All these buttons of the toolbar function in somewhat the same way; you click on a button and then use the mouse to either select one or more objects (when the **Select Mode** ( ) button was clicked) or create the corresponding visual object. Notice that after you click on one of these eight buttons, the button stays depressed and when you move the mouse over the workplace area, the mouse cursor becomes:

if the **Select Mode** ( ) button is pressed ('Select Mode'), or

if the **Text Mode** (T) button is pressed ('Text Mode'), or

if any of the other six buttons are pressed ('Visual Objects Mode').

▶ When in 'Select Mode'...

When you are in 'select mode', then the mouse cursor changes to a 'select mode' cursor to remind you that may go over any object (visual or processing) and click on it, in order to select it. If you need to add other objects in the selection set, you may click on them by holding the **Ctrl** key down. If you **Ctrl+Click** on an object that is already selected, then the object is removed from the selection set. If you plan on selecting many objects, you may opt to 'group-select' them by drawing a "lasso" around them. The "lasso" can be drawn by pressing the left button on an empty area and dragging the mouse until the rectangle displayed on the screen with a dotted-line as a border is large enough to include all the elements that you want included in the selection set. When you let go of the mouse button, all the objects that are fully included in the "lasso" area will be displayed as selected.

▶ When in 'Text Mode'...

When you are in 'text mode', then the mouse cursor changes to a 'text mode' cursor to remind you that you are about to insert a text object.

▶ When in 'Visual Objects Mode'...

When you are in 'visual objects mode', then the mouse pointer changes to a 'visual objects mode' cursor to remind you that you are about to insert a visual object.

13.2a Text Object

▶ To Insert a Text Object...

1. Click on the text mode button T on the Visual Objects Toolbar.
2. Move the mouse to the location where you want to start typing the text and click.
3. Notice how the system inserts automatically the string "Text" that is already highlighted so that as you start typing the text is replaced by your typing.
4. When you are done typing, you may click anywhere away from the object.

Notes:

(a) During the typing of the text, most of the system services are temporarily suspended (notice how most of the main menu entries are disabled).

(b) The text typed can contain carriage-return characters (i.e., the text can be a multi-line text). Simply hit **Enter** to insert a new line character.

(c) During typing, you may use the arrow keys to move the cursor. You can select text pieces either by moving the cursor with the arrow keys while holding down the **Shift** key or by click-and-dragging the mouse. As usual, **Ctrl+X** or **Shift+Del** cuts the selected text, **Del** or **Backspace** erases the selected text, and **Ctrl+V** or **Ctrl+Ins** or **Shift+Ins** inserts the text kept in the clipboard.

(d) If, during typing, you decide to abort the creation of this new text object, simply hit the **Esc** key.

(e) You can modify the appearance of the text by editing its style (font specification, text color, background color and frame, see Editing the Style of Visual Objects).

(f) All text on the flowsheet can be viewed and edited in a tree-like structure on the Documentation Toolbar Process node.

(g) A text object can be hidden by right clicking on the text and selecting **Hide Text**. Once a text object is hidden a Post-It Note icon is displayed in its place with a label below it (NOTE-x) (x is an integer number incremented by the number of text objects on the flowsheet. The label name can also be edited). The text can still be viewed as a tooltip when the mouse hovers over the icon. Hiding text can help the user un-clutter the flowsheet of very large text objects. The text can be shown again by right clicking the icon and selecting **Show Text**.

13.2b Line

▶ To Insert a Line...

1. Click the **Line** button on the Visual Objects Toolbar.
2. Move the mouse to a location where you wish to start drawing the line and click once.
3. Move the mouse to the other end of the line and click again.

Notes:

(a) To insert a line that is either horizontal or vertical, make sure that you hold down the **Shift** key during the mouse move (step 2 above). Then the system automatically draws either a horizontal or vertical line (whichever is closer to the location of the mouse cursor).

(b) If, during the drawing of a line, you decide to abort, then simply hit **Esc**.

(c) You can modify the appearance of the line by editing its style (line thickness, style, color, see Editing the Style of Visual Objects).

13.2c Rectangle, Round Rectangle or Ellipse

▶ **To Insert a Rectangle / Round Rectangle / Ellipse or Circle...**

1. Make sure the corresponding button is clicked on the Visual Objects Toolbar.
2. Move the mouse to the top-left corner of the desired location of the object you are inserting (which, in the case of drawing an ellipse, would be the top-left corner of the ellipse's enclosing rectangle).
3. Hold down the left mouse button and drag the mouse. Notice how the shape and size of the inserted object follows the cursor as it moves.
4. When, the object has the desired size, release the mouse button.

Note:

(a) To insert an object with fully symmetrical shape (i.e., a square or an ellipse) make sure you hold down the **Shift** key before the first mouse click (in step 3 above). Then, the system automatically draws a square or a circle (instead of following the mouse cursor precisely).

(b) You can modify the appearance of the rectangle by editing its style (line thickness, style, interior color, see Editing the Style of Visual Objects).

13.2d Polyline or Polygon

▶ **To Insert a Polyline / Polygon...**

1. Make sure the corresponding button is clicked on the Visual Objects Toolbar.
2. Move the mouse to a location where you wish to locate the first vertex of the polyline / polygon and click.
3. Move the mouse to the location of the next vertex of the polyline / polygon and click. Repeat until you have created all the vertices of the polyline / polygon.
4. To end the drawing of the polyline / polygon, double-click to enter the last vertex.

Notes:

(a) During the insertion of vertices, a right-click will cancel the last vertex inserted.

(b) If during the drawing of a polyline / polygon, you decide to abort, then simply hit **Esc**.

(c) After you have drawn a polyline or polygon, you can edit (relocate) any of its segment corners by selecting the polyline/polygon and then selecting the Reshape option from its context (right-click) menu (as a shortcut you can simply double-click on the polyline or polygon). Notice that a handle appears on every corner point of the line. You can drag these handles to any location desired.

(d) You can modify the appearance of the polyline or polygon by editing its style (line thickness, style, color, see Editing the Style of Visual Objects).

13.3 EDITING EXISTING VISUAL OBJECTS

Before we edit any object, we must select it. Make sure you are in 'select mode' and click on the object that you want to edit. Notice that:

- if the object is a text object, then it is displayed in red color with a dotted frame around it, and
- if the object is any of the other types of visual objects, then a set of black square rectangles (called 'handles') are displayed.

▶ To Edit a Text Object...

1. Move the cursor over the text and right-click. From the context-menu that appears select **Edit**.
2. Move the insertion point anywhere in the text you need to make changes or insert new text.
3. To end the editing of the text object, simply click anywhere outside the area of the text.

Notes:

(a) As a short-cut to step 1 above, you may simply move the cursor over the text object that you wish to edit and double-click on it.

(b) If, during the editing of a text object, you decide to abort and keep the text with its old contents, simply hit **Esc**.

▶ To Edit (Resize) Any Visual Object (Except Text)...

1. Click on the desired object to select it.
2. Move the mouse over one of the selection handles and drag the handle. Notice how the visual object's size changes to re-fit itself within the new rectangle established by the new location of the handle.

Notes:

(a) The handles displayed on the middle point of an surrounding rectangle's edge allow you to move that side only. The corner rectangles allow you to move two sides at the same time.

(b) Polylines and polygons can be resized just like any other visual object. Resizing a polygon or a polyline essentially scales up or down the dimensions of every edge and appropriately adjusts the location of the vertices. If you want to simply move the location of the vertices but not affect the entire size of the polyline / polygon, see the instructions on how to reshape a polyline or polygon that follow.

(c) If more than one objects are included in the selection set and a selection handle is being dragged, then the entire set of objects get resized.

▶ **To Reshape a Polyline or a Polygon...**

1. Click on the desired polyline or polygon to select it.
2. Right-click on the selected object and click **Reshape** on the command menu that appears (see 13.4 Visual Objects Command Menu).
3. Move the mouse over the vertex that you wish to move and drag its handle to the desired new location.
4. Repeat with all vertices that you wish to relocate.
5. To end the reshaping of the polyline / polygon, simply click away from the object.

Notes:

(a) During the reshaping of a polyline / polygon all other user options are being temporarily disabled (until the end of the reshaping session).

(b) Unlike resizing, reshaping can only be applied to one object (polyline or polygon) at a time.

13.4 VISUAL OBJECTS COMMAND MENU

Just like any object that is part of a process file, visual objects can accept certain commands that affect their appearance. To see the menu of commands accepted by a visual object, you can simply move the mouse over the object and right-click, to invoke its context menu. Even though the exact list depends on the type of visual object that you are addressing, the following commands are accepted by almost all visual objects (see Note (a) below for exceptions):

- Rotate {Left or Right}
- Flip {Horizontal or Vertical}
- Order {Bring Forward, Send Backward, Bring to Front, Send to Back }
- Style {Pick Up, Apply Style, Edit Style, Use Default}

All of the above commands can also be administered from the Visual Objects toolbar's last ten buttons (see 13.5 Visual Objects Toolbar). Each command is described below:

- **Rotate Left / Right...**

  Applying this command to the selected object(s) will rotate them left / right by 90°.

- **Flip Horizontal / Vertical...**

Will rotate the selected object(s) by 180° around a hypothetical horizontal / vertical axis.

- **Bring Forward / Send Backward...**

  As several objects are drawn on the workspace area, it is possible that one may partially (or totally) overlap another. The order by which objects are drawn determines which object gets to be displayed last and therefore be exposed in its entirety. Move advances the selected object(s) by one position in the drawing order and relative to all other objects that currently exist in the process file (including procedure icons and streams). The further an object is moved the more exposure is likely to get when displayed. The further back an object is sent, the more of its surface could be covered by other objects that will be drawn after it. Note that if more than one objects are selected to move forward or backward in the drawing order, their relative position remains unchanged.

- **Bring To Front / Send To Back...**

  Sending an object to the front, will make sure that the object will be drawn last and therefore it will completely exposed to view. The opposite will happen when we send an object to back. In the latter case, if any other objects are partially or totally overlapping with it, they will get to be shown on top of the object moved to back. Note that if more than one objects are selected and sent to front or back, their relative position in the drawing order remains unchanged.

- **Pick Up Style...**

  Besides location and size, style also affects the appearance of every visual (as well as processing) object. The elements that constitute the drawing style of an object depend on the object's type. For example, for lines, the line color, the presence or absence of arrowheads at the end and the beginning of the line and the line thickness are the only style components. In rectangles, ellipses and other solid objects, the fill-in characteristics are also components of their style. For text objects, on the other hand, none of the above is part of their style. Instead, the font name, font size and text color are part of a text object's style. For more on how to set the style characteristics of a visual object or how to set the default style for all visual objects, see in the following section (Editing the Style of Visual Objects).

  In any case, the style of an object is the collection of all characteristics that determine the visual appearance of an object (other than position and size). By selecting an object and clicking on the palette's button that correspond to this command, copies all of its style's characteristics. Typically, a pick up style command will be followed by one or more apply style commands that actually apply the copied style to one or more target objects, thereby making their visual characteristics identical to the source object.

- **Apply Style...**

  Once the style of an object has been picked up (see above), then we can select others (of the same or similar type) and apply the selected style on them.

Notes:

(a) Commands **Rotate Left / Right** and **Flip Horizontal / Vertical** don't apply to text objects.

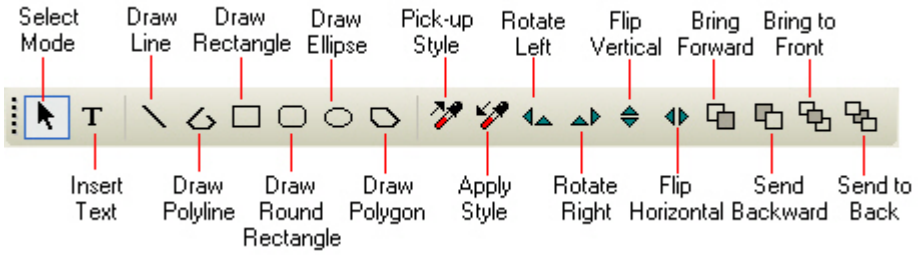
(b) If multiple objects are selected, invoking a context-menu command will include only the entries that are common to all object types selected (and therefore, the only options that can be applied to all the objects selected).

(c) Just like visual objects, procedure icons and process streams also have a style: the style of a procedure's icon is made up of the icon's color, its tag's font and color, and its description label font and color. Similarly, a stream's style is made up of its own color as well as its tag's font and color. The style of procedures and streams can be picked up and applied just like any other visual object.

(d) If you picked-up the style of an object and then applied it to others whose attribute styles are sub/super-sets of the source object, only the applicable style components (if any) will be copied. For example, if you picked up the style of line object and applied it to a solid object (like a rectangle) only the rectangle's line characteristics will change to match the source's line characteristics. On the other hand, if you applied the picked up style of a rectangle to a line, the reverse will happen. The line characteristics will be taken on by the target line and the fill-in characteristics will be ignored.

13.5 VISUAL OBJECTS TOOLBAR

The following toolbar is shown by clicking **Toggle Visual Objects Toolbar** ( ) on the **Main** toolbar, or by selecting **Visual Objects Toolbar** on the **View** menu, or by right-clicking on any toolbar and selecting **Visual Objects** on the shortcut menu that appears:



Each button is described below:

- The **Select Mode** ( ) button sets the mouse cursor to 'Select Mode'. In this mode, mouse clicks can be used to select objects on the flowsheet.
- The **Text Mode** ( ) button sets the mouse cursor to 'Text Mode'. In this mode, the next mouse click will be used to insert text in the flowsheet.

The next six buttons set the mouse cursor to 'Visual Objects Mode'. When clicked, the mouse cursor will change to inform you that you are about to "Add a Visual Object". The following objects are supported:

- The **Line** ( ) button enables you to draw a straight line.
- The **Polyline** ( ) button enables you to draw a polyline.

- The **Rectangle / Square** ( ) button enables you to draw a rectangle or square (if you hold down the **Shift** key while drawing).
- The **Round Rectangle / Square** ( ) button enables you to draw a round rectangle or square (if you hold down the **Shift** key while drawing).
- The **Elliplse / Circle** ( ) button enables you to draw an ellipse or circle (if you hold down the **Shift** key while drawing).
- The **Polygon** ( ) button enables you to draw a polygon.

To learn how to do draw the above visual objects, see 13.2 Adding a New Visual Object. After you draw an object, you can move its vertices (see 13.3 Editing Existing Visual Objects) and you can also change its style (color, thickness, etc.) (see 13.6 Editing the Style of Visual Objects).

- The **Pickup Style** ( ) button allows you to quickly pick up (copy) the whole style of any object on the flowsheet (so that you can apply it to others later). Just select the object whose style you wish to copy and then click on the button shown next.
- The **Apply Style** ( ) button will apply a picked up (copied) style to the set of objects currently selected. It is only active if you have picked up a style previously and the set of currently selected objects is compatible to the style copied earlier.
- The **Rotate Left** ( ) button will rotate the set of selected visual objects by 90º to the left. It is only active if some visual objects (that can be rotated) are currently selected. Note that procedure icons, streams and text objects cannot be rotated.
- The **Rotate Right** ( ) button will rotate the set of selected visual objects by 90º to the right. It is only active if some visual objects (that can be rotated) are currently selected. Note that procedure icons, streams and text objects cannot be rotated.
- The **Flip Vertically** ( ) button will flip the set of selected visual objects vertically (i.e., around a horizontal axis). It is only active if some visual objects (that can be flipped) are currently selected. Note that procedure icons, streams and text objects cannot be flipped.
- The **Flip Horizontally** ( ) button will flip the set of selected visual objects horizontally (i.e., around a vertical axis). It is only active if some visual objects (that can be flipped) are currently selected. Note that procedure icons, streams and text objects cannot be flipped.
- The **Bring Forward** ( ) button will set the selected object(s) forward one position in the display order. When two objects overlap each other, the object in front (in the order) will show on top.
- The **Send Backward** ( ) button will set the selected object(s) backward one position in the display order. When two objects overlap each other, the object in the back (in the order) will show behind.
- The **Bring To Front** ( ) button will set the selected object(s) forward to the front of the display order.

- The **Send To Back** ( ) button will set the selected object(s) backward to the back of the display order.

13.6 EDITING THE STYLE OF VISUAL OBJECTS

The attributes that comprise the style of a visual object depend on the object type. The style attributes of shapes affect the appearance of:

- the lines (thickness, color, arrow-heads)
- the interior - for solid objects only - (solid color, pattern or none)

On the other hand, the style attributes for text objects affect:

- the text font (type, size, boldness, etc.)
- the text color

Note that process step icons have their own style. Their style affects:

- the color of the icon
- the color of their labels (process step name, equipment name, and description)
- the font of their labels (process step name, equipment name, and description)
- the visibility of their labels (process step name, equipment name, and description)
- the style, color and thickness of the label frames line

Similarly, streams have a style that affects:

- the color of the lines
- the thickness of the lines
- the color of the stream's label
- the font of the stream's tag
- the visibility of the stream's tag
- the style, color and thickness of the label frame line

▶ To Edit the Style of a Visual Object...

1. Move the cursor over the object, right-click on it to bring-up the context menu and select **Style ▸ Edit Style**. This will bring up the object's style dialog (the Text Style Dialog for text, or the Line Style Dialog dialog for a line or polyline, or the Shape Style Dialog for all other visual objects) through which you can modify all the attributes of the selected object.
2. Make any choices that you wish to apply in the selected object's style and click **OK**.

If you select **Style ▸ Use Default**, then the selected object(s) will be forced to follow the style set as the default style of such objects. To find out how to edit the default style of visual objects, see 13.6a Editing the Default Style of Visual Objects.

13.6a Editing the Default Style of Visual Objects

Every visual object that is inserted into a process file must be provided with a style (default style). The characteristics of the default style can be edited for each process file. Note that the changes will stay saved with the saved process file and the next process file will use the defaults that your software has built-in.

▶ To Edit the Default Style for Text Objects...

1. Select **Preferences ▸ Default Styles ▸ Text** either on the **Edit ▸ Process Options** menu or on the right-click menu of the flowsheet. A dialog similar to the Text Style Dialog will be displayed.
2. Make your selections for all style attributes and click **OK**.

▶ To Edit the Default Style for All Other Visual Objects...

1. Select **Preferences ▸ Default Styles ▸ Text** either on the **Edit ▸ Process Options** menu or on the right-click menu of the flowsheet. A dialog similar to the Line Style Dialog will be displayed.
2. Make your selections for all style attributes and click **OK**.

14 EXCHANGING DATA WITH OTHER APPS

No matter how many features we can pack into our software, it is impossible to expect that a user will accomplish everything their daily job requires using only one tool. It is rather common to expect to have an arsenal of software tools, each specializing in its own domain and one can only hope that they can work cooperatively and smoothly with each other, allowing a user to accomplish his/her goals. In that spirit, SuperPro Designer allows you to export a variety of information related to your simulation project (such as pictures, numbers alone or in tables or even entire reports) to several applications running under the MS-Windows® operating system (such as word processors, spreadsheets, or more advanced graphic editors). More specifically, you can:

- Export process flowsheet drawing (see 14.1a Exporting Process Flowsheet Drawing) and charts (see 14.1b Exporting a Chart Drawing).
- Export all the reports in a variety of formats (MS-Word, HTML, etc.), see Reports.
- Export all the scheduling and resource consumption data (for a batch recipe) to MS-Project® (see 14.2c Exporting Scheduling & Resource Consumption Data to MS-Project) and SchedulePro (see 14.2d Exporting Scheduling & Resource Consumption Data to SchedulePro), MS-Excel® (see 14.2a Export Process Scheduling Data to MS-Excel and 14.2b Export Resource Consumption Data to MS-Excel).
- Export selected process information displayed on a grid (e.g. a given equipment's contents, the stream summary table, a selected procedure's activity overview table, etc.), to a MS-Excel® spreadsheet. The exported grid can also be hot-linked with SuperPro Designer so that it is automatically updated if the contents change (see 14.3 Exporting / Linking Tables (Grids) to MS-Excel).
- Use the application as a COM server (from another COM friendly computing environments such as MS-Excel® scripting, C++ or C# applications, etc.) to load a process file, access most of the information in the file, change values and redo the M&E balances, economic calculation, generate and export charts, etc. (see 14.5 Using SuperPro Designer's OLE Server).

Besides exporting its own information, the application allows you to insert in the flowsheet foreign objects (e.g. spreadsheets, bitmaps, etc.) as OLE objects pasted (or linked) into the process flowsheet (see 14.4 Importing OLE Objects).

14.1 EXPORTING FLOWSHEET & CHART DRAWINGS

SuperPro Designer is an invaluable tool in representing a process (especially in its early stages) and evaluating several alternatives by performing 'what-if' experiments. Almost always, an engineer will eventually have to collect the results of such experiments and put them together in a report that will be submitted to his/her colleagues or supervisor. The application allows you to integrate all the drawings you have created and the results that you have generated very easily into your reports. Also, if the scope of the process simulation was only for a preliminary analysis and, after approval, a more detailed process drawing is expected to be done using more process drawing tools (such as AutoCAD®) it is possible to export the flowsheet drawing to an AutoCAD®-compatible format so that it can be used as a seed for the further process enhancements. In this section, you will find out how you can:

(a) Incorporate the entire flowsheet drawing or sections of it into other programs (see 14.1a Exporting Process Flowsheet Drawing).

(b) Incroporate charts (as pictures) generated by the software into your reports (see 14.1b Exporting a Chart Drawing).

14.1a Exporting Process Flowsheet Drawing

There are two possible ways that you can export flowsheet drawings and later incorporate them into another program:

1. Using the clipboard (aka, cutting-and-pasting).
2. Using a file to store the picture and later import it from the other application.

EXPORTING THE PROCESS FLOWSHEET USING THE CLIPBOARD

This is probably the most commonly used method for sharing either the entire picture of a flowsheet, or just a section of the flowsheet drawing with another application.

▶ **To copy-and-paste the flowsheet (whole or parts) using the clipboard...**

1. Make sure that you are in select mode (the button is pressed o the main toolbar). Click-and-drag the mouse to create a selection rectangle large enough to include all the elements that you wish to be included. Shift+Click to include (or remove) more elements (one-by-one). If the entire flowsheet needs to be copied, you may choose **Edit ▸ Select All** (or **Ctrl+A** as a shortcut) in order to select the flowsheet in its entirety.
2. Copy the selected parts to the clipboard
   Select **Edit ▸ Copy** from the application's main menu (or **Ctrl+C** as a shortcut, or click on the **Copy** button ( ) of the main toolbar.
3. Paste the clipboard contents into the receiving application
   Bring up the program where you want to include the drawings (e.g., MS-Word®) and open the document (report) that you wish to include the flowsheet drawing. Find the **Edit** menu. You will have two choices:
   a) Select **Paste** (or type **Ctrl+V** or **Ctrl+Ins**, or click on the paste button ( )
   b) Select **Paste Special**. The dialog shown in Figure 14.1 will appear (actual contents of the list in your environment may be different). Notice that you have two decisions to make in this dialog. The first decision refers to the nature of the pasted object as it will continue

to exist in the receiving application. Your choices are displayed in the listbox:
(a) 'SuperPro Designer Flowsheet Object', or
(b) 'Picture'
If you select 'Picture', then the pasted object will be treated as a plain picture and most word processors (or spreadsheets) will allow you edit the picture locally, in case you need to add and/or remove anything to it (e.g. comments or highlights). If you select 'SuperPro Designer Flowsheet Object', then you can only edit the picture only if you (or the viewer of the report) has a copy of SuperPro Designer installed. will be able to edit the contents of the pasted picture. If you choose to include the picture as a 'SuperPro Designer Flowsheet Object' then you can either have the picture:
(a) Pasted, or
(b) Paste-Linked
into the receiving document. There is a significant difference between options (a) or (b) above. Choosing (b) implies that there will continue to be a ´live´ connection (sometimes referred to as ´hot-connection´) between the receiving document and the source of the pasted image (SuperPro Designer's process file). If you modify the contents of the source file, then the image in the receiving document will change as well to reflect the most current version of the process file. However, this behavior sometimes may not what you want. Instead you may want to insert a ´frozen´ picture of the design case as is now, and not have it change later. In this case you must choose (a) (i.e., simple pasting).The disadvantage of a live-link ('Paste-Link') is that the viewer of the report must have access to the original process (.spf) file and they must also have a copy of the application installed in order to view the report.

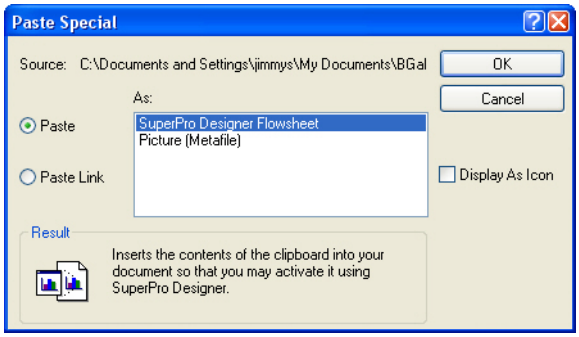


Figure 14.1: The 'Paste Special' dialog.

The option to include the copied flowsheet picture as a 'SuperPro Designer Flowsheet Object' will not be there if the clipboard only holds a partial description of the original flowsheet. You must have placed the entire flowsheet on the clipboard in order to be able to paste (or paste-link it) as a 'SuperPro Designer Flowsheet Object'.

PASTING INTO ANOTHER SUPERPRO DESIGNER DOCUMENT

It is perfectly legal to paste the flowsheet (or its parts) placed into the clipboard into another SuperPro Designer process flowsheet. When this is done, the application will insert all the copied procedures and streams into the destination flowsheet. There are many actions that the application will take in the background when this happens and that users should be aware:

1. Before the insertion of the copied unit procedures and streams, the application will check to verify that all components and mixtures present in the source document (where the flowsheet parts where copied from) are also present in the destination flowsheet. If that is not the case, then before the insertion of the copied objects is made, the list of registered components and mixtures will be automatically expanded to include the missing items (components and mixtures that existed in the source document but not in the destination document). Make sure that when you paste the flowsheet, the original source document is still opened within SuperPro Designer. The application will identify the existence of such ingredients by their local names. If you have inadvertently named a different component (or mixture) in the destination flowsheet with the same local name as the source flowsheet, the copied information will not be as you expected. That is another reason why you should choose the local names of components and mixtures very carefully during their registration.
2. The same cross-registration of entities will happen for any heat transfer agents, labor types, power types, or any other resources used in the source flowsheet but not in the destination flowsheet. Once again, for resources that were locally introduced in the source and destination flowsheets (i.e. they were not copied from the databanks) there is a possibility of a mix-up, if the same name has been chosen to represent to different resources.
3. All scheduling references of operations will be reset to the default choice: for the lead operation the reference will be reset with respect to the beginning of the batch, and for the follow-up operations in a procedure, their scheduling reference will be with respect to the end of the previous operation in the queue. All external references will be eliminated as it cannot be guaranteed that such operations are part of the copied set. The lead/lag values (time shift) will be left as is.

Since several alteration can be made during the pasting of a flowsheet into another flowsheet, it is not recommended practice to build a large process in pieces and then copy-and-paste the parts together to represent the entire process. The two acceptable alternatives would be to: (a) gradually keep adding to the process file all elements till the entire process is represented or (b) build the different parts of the process in different process files and use the auto-initialization of streams (see 4.9 Auto-Initialization of Input Streams) or equipment contents (see 6.15j Initial Equipment Contents: Initialization Options Dialog) feature to connect the files together.

EXPORTING THE PROCESS FLOWSHEET IN A METAFILE (WMF)

Most graphics applications and word processing applications allow you to insert in their document a picture as contained in a file. By far, the most popular graphics format in the Windows® world is the "Windows Metafile" format, or "wmf" format for short. It is very popular because it allows graphics to be saved and later inserted within a frame of a given size with minimal distortion of picture quality. Furthermore, several of the leading word processing and graphics applications, can recognize graphic elements in a "wmf" graphic and allow users to edit the picture using their own picture editor. MS-Word®, for example, has its own metafile picture editor. Therefore, you can insert a picture into MS-Word® from a "wmf" file, resize it, edit it and later save it again as part of the MS-Word® document. SuperPro Designer allows you to export the drawing of a process flowsheet in a Windows Metafile format.

▶ To export the flowsheet (whole or parts) as a metafile...

1. Select the part that you wish to copy (or the whole flowsheet)
   Make sure that you are in select mode (the button is pressed o the main toolbar). Click-and-drag the mouse to create a selection rectangle large enough to include all the elements that you wish to be included. Shift+Click to include (or remove) more elements (one-by-one). If the entire flowsheet needs to be copied, you may choose **Edit ▸ Select All** (or **Ctrl+A** as a shortcut) in order to select the flowsheet in its entirety.
2. Export the selected items into a 'wmf' file
   Select **File ▸ Export Items to Metafile** from the application's main menu. A file selection dialog will appear, prompting you to select a location (folder) and a name to be used. Type in the filename that you wish to contain the description of the flowsheet in "wmf" format. By convention, all such files should have a ".wmf" extension. The file need not already exist. In fact, if the program discovers that a previous file exist with the same name and in the same location on your hard disk, it will ask for your permission to overwrite it.
3. Import the 'wmf' picture in the receiving document.
   The actual menu selection may differ (depending on the receiving application). Typically there will be a **Insert ▸ Picture ▸ From File** menu option (for the exact menu option please consult your software's manual or online help). Select the file as set by the previous step (2).

*If no items (procedures, streams, visual objects, etc.) are selected in your flowsheet, the command **File ▸ Export Items to Metafile** will be shown as disabled.*

EXPORTING THE PROCESS FLOWSHEET AS A (DXF) AUTOCAD® FILE

AutoCAD® is a popular detailed engineering software package, used by several companies to produce detailed Process & Instrumentation (P&I) Diagrams. Even though the flowsheet representation in SuperPro Designer is usually not detailed enough to qualify directly as a P&I diagram, it can be used as a starting seed for creating the detailed P&I diagram for a process. Consequently, some users will find it very useful the fact that they can export the entire flowsheet or parts of it into a file that is in DXF format (that is the vector graphics format used by AutoCAD®). Besides AutoCAD®, several other graphics packages (like Visio®, CorelDraw®, etc.) will allow you to import graphics in this format and later convert the drawing into their own native format.

▶ To export the flowsheet (whole or parts) as a DXF file...

1. Select the part that you wish to copy (or the whole flowsheet)
   Make sure that you are in select mode (the button is pressed o the main toolbar). Click-and-drag the mouse to create a selection rectangle large enough to include all the elements that you wish to be included. Shift+Click to include (or remove) more elements (one-by-one). If the entire flowsheet needs to be copied, you may choose **Edit ▸ Select All** (or **Ctrl+A** as a shortcut) in order to select the flowsheet in its entirety.

2. Export the selected items into a 'dxf' file
   Select **File ▸ Export Items to AutoCAD®** from the application's main menu. A file selection dialog will appear, prompting you to select a location (folder) and a name to be used. Type in the filename that you wish to contain the description of the flowsheet in "dxf" format. By convention, all such files should have a "dxf" extension. The file need not already exist. In fact, if the program discovers that a previous file exists with the same name and in the same location on your hard disk, it will ask for your permission to overwrite it.
3. Import the drawing from AutoCAD® or other 'dxf' friendly software.
   Typically there will be a **File ▸ Open** menu that will allow you to open a '.dxf" file. Make sure that in the file format displayed '*.dxf" or '*.*' is selected. Locate the file as specified in step (2) above and open it.

*If no items (procedures, streams, visual objects, etc.) are selected in your flowsheet, the command **File ▸ Export Items to AutoCAD®** will be shown as disabled.*

Only the drawing of the flowsheet is exported in the DXF file. None of the data behind the icons (unit procedures, operations, equipment or streams) are exported. Also, remember that when SuperPro Designer drawings are exported into 'dxf' format, the images are converted to a set of elemental shapes (lines etc.) but they are not grouped into compound objects. This should be done from the receiving application (AutoCAD®, CorelDraw®, etc.) at a later stage.

14.1b Exporting a Chart Drawing

You can export any chart (as a picture) from SuperPro Designer into another Windows® application (e.g. a word processor). The export can happen with one of two ways:

1. Using the clipboard (aka, cutting-and-pasting)
2. Using a file to store the picture and later import it from the other application.

▶ To copy a chart using the clipboard...

1. Generate a chart of your choice (the equipment occupancy chart, the operations gantt chart, any resource consumption chart, etc.)
2. Copy the chart into the clipboard
   From the chart's command (context) menu, select **Copy**. The chart's context menu appears when your right-click on an unoccupied area of the chart.
3. Paste the chart in the destination document
   Open the document where you wish to paste the chart (MS-Word® document, or MS-Excel® spreadsheet, etc.) and select **Edit ▸ Paste** from the application's main menu (usually, **Ctrl+V** can be used as a shortcut). Note that **Paste Special** and the options available to OLE items does not apply to charts; they can only be pasted as pictures and not paste-linked as OLE objects.

▶ **To copy the chart as a metafile (".wmf" file)...**

1. Generate a chart of your choice (the equipment occupancy chart, the operations gantt chart, any resource consumption chart, etc.).
2. Save the file into a '.wmf' file
   From the chart's command (context) menu, select **Export Chart as Metafile**. The chart's context menu appears when your right-click on an unoccupied area of the chart. This will bring up a typical file selection dialog from where you can specify the location (folder) and file name to be used for the storage of the chart as a Windows Metafile. By convention, all such files should have a ".wmf" extension. The file need not already exist. In fact, if the program discovers that a previous file exist with the same name and in the same location on your hard disk, it will ask for your permission to overwrite it
3. Import the 'wmf" chart (as a picture) in the receiving document.
   The actual menu selection may differ (depending on the receiving application). Typically there will be a **Insert ▸ Picture ▸ From File** menu option (for the exact menu option please consult your software's manual or online help). Select the file as set by the previous step (2).

14.2 EXPORTING PROCESS DATA

SuperPro Designer allows you to export various process data (resource consumption/inventory, scheduling information, etc.) in various ways:

- Export Process Scheduling Data to MS-Excel
- Export Resource Consumption Data to MS-Excel
- Exporting Scheduling & Resource Consumption Data to MS-Project
- Exporting Scheduling & Resource Consumption Data to SchedulePro

14.2a Export Process Scheduling Data to MS-Excel

If you need to export all the data associated with the scheduling of all operations in your process (start time shift, process time, turnaround time, etc.) the application allows you to create an "xls" (Excel® formatted) file that contains all this information. Here is how you can generate that file:

▶ **To export scheduling data to MS-Excel®...**

1. Bring up the gantt chart for operations (see 7.4 The Operations Gantt Chart (OGC)) or for equipment (see 7.5 The Equipment Gantt Chart (EGC)) or the equipment occupancy chart (see 7.6 The Equipment Occupancy Chart (EOC)).
   To bring up the operations gantt chart, select **Tasks ▸ Gantt Charts ▸ Operations GC ▸ ...** from the main menu of the application; to bring up the equipment gantt chart select **Tasks ▸ Gantt Charts ▸ Equipment GC ▸ ...** from the main menu of the application; to bring up the equipment occupancy chart, select **Charts ▸ Equipment Occupancy ▸ ...**.

2. Select **Export Data to Excel**
   From the chart's command (context) menu, select **Export Scheduling Data to MS-Excel®**. The context menu for the chart appears when you right-click over an unoccupied area of the chart. The file selection dialog will come up. Select a location (folder) and a file name where you wish to have the data saved. By convention, MS-Excel® files have an 'xls' extension. The file need not already exist. In fact, if the program discovers that a previous file exist with the same name and in the same location on your hard disk, it will ask for your permission to overwrite it.
3. Open the file from MS-Excel®
   Start MS-Excel®, and select **File ▸ Open**. Locate the file that you specified in step (2) above. Some minor column formatting may be necessary for all the values to appear properly.

14.2b Export Resource Consumption Data to MS-Excel

The most common motivation for exporting resource consumption data to MS-Excel is when a user needs to combine consumption information (for the same resource) from different recipes. Since a SuperPro Designer recipe typically only focuses on one product at a time but at the same time, several recipes may be forced to share common resources in the same production site (e.g. heat transfer agents, material supplies, labor, etc.) it may be vital to combine the consumption from several recipes (with overlapping execution times) to make sure that any rate supply or cumulative supply limit are not violated. For example, a steam distribution system may have a built-in limitation (upper limit) as to how much steam can be distributed at a given time (in kg/h or lb/s). Storage limitations may place an upper limit as to how much a given buffer can be consumed in the span of 12 hours (between replenishing runs). SuperPro Designer makes it easy to check against such resource constraints when a single process is assumed to be running. However, when consumption is supposed to be combined from different recipes (running at overlapping times) you must combine the consumption data from each recipe. Bringing the data from each recipe into an Excel® file and later combining the numbers is a relatively easy way to accomplish this task.

When combining the batch execution data from multiple recipes (assuming multiple batches from each recipe) remember that SuperPro Designer assumes that each batch (of the same recipe) repeats itself in an identical fashion only with a time shift from the one before it (the recipe's cycle time). In reality, due to practical constraints, this may not be the case. Some follow up batches may be late to start, or some operations in a later batch may not start in exactly the same time shift from the batch start. For better flexibility in representing batches and understanding resource constraints as they originate from multiple batch executions from the same or multiple recipes in the same site, it is strongly recommended to export the data into SchedulePro (see 14.2d Exporting Scheduling & Resource Consumption Data to SchedulePro) and perform the resource debottlenecking analysis there.

▶ To export resource consumption & inventory data to MS-Excel®...

1. Bring up the resource consumption or inventory chart for the desired resource (material, heat transfer agent, labor, power)
   To generate the resource consumption / inventory chart, select the appropriate entry in the **Charts ▸ Materials ▸ ...** or **Charts ▸ Labor ▸ ...** or **Charts ▸ Heat Transfer Agents ▸ ...** or **Charts ▸ Power ▸ ...** menu from the application's main menu.

2. Select **Export Data to MS-Excel®**.
   From the chart's command (context) menu select **Export Data to MS-Excel®**. The context menu for the chart appears when you right-click over an unoccupied area of the chart. The file selection dialog will come up. Select a location (folder) and a file name where you wish to have the data saved. By convention, MS-Excel® files have an 'xls' extension. The file need not already exist. In fact, if the program discovers that a previous file exist with the same name and in the same location on your hard disk, it will ask for your permission to overwrite it.
3. Open the file from MS-Excel®
   Start MS-Excel®, and select **File ▸ Open**. Locate the file that you specified in step (2) above. Some minor column formatting may be necessary for all the values to appear properly.

14.2c Exporting Scheduling & Resource Consumption Data to MS-Project

If you are accustomed to using MS-Project® for your scheduling representations (especially if you need to add real-calendar-based scheduling capabilities to batch processes developed by SuperPro Designer) you will appreciate SuperPro Designer's MS-Project® Export facility. This facility exports to an XML format that can be directly imported by MS-Project®, all the operation scheduling and resource consumption data from a recipe. Furthermore, from MS-Project®, you can import (in the same project) data from different recipes so that they can be combined and analyzed in order to identify potential bottlenecks.

Exporting scheduling and resource data through MS-Project® offers several advantages over MS-Excel®:

- Scheduling links among operations (e.g. start-to-start, start-to-finish, etc.) are retained in MS Project®
- Multiple batch export is supported
- Staggered equipment operation is supported
- Equipment, labor, power and material resources are automatically defined in MS Project®
- Equipment utilization, power consumption and material and heat transfer agent utilization levels are also included in the export file.

ABOUT THE EXPORT PROCESS

SuperPro Designer now communicates its data to MS-Project® by exporting it to an XML file formatted specifcally for MS-Project®.

Operations are exported as fixed duration tasks. Procedures and sections are exported as summary tasks. Equipment and labor are exported as work-resources. All other resources are treated as material resources.

▶ To Export Scheduling & Resource Consumption Data to MS-Project®...

1. Select the **File ▸ Export to MS-Project® XML File** command (from main menu) or from the operations gantt chart interface by selecting **File ▸ Export to MS-Project® XML File** from the menu or by selecting **Export to MS-Project® XML File** from the chart's command (context) menu. The following dialog (Figure 14.2) will appear:

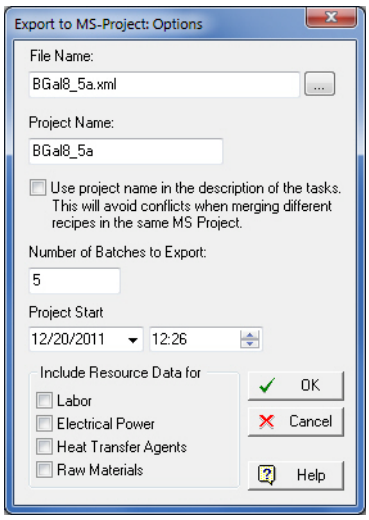


Figure 14.2:The 'Export to MS-Project® dialog.

2. Select the information that you wish to export and provide a name for the recipe
From this interface you can select the file name of the exported xml file. Also it allows you to customize the content of the data being exported as well as give them a name (project name, or recipe name) that will be listed in MS-Project®. You can set the number of batches for which data is to be exported as well as whether you wish to include resource consumption data (i.e. for labor, electrical power, heat transfer agent and/or raw materials). Finally, you must specify a date/time to be kept as the calendar start time of the exported project. For details, see Export to MS-Project Options Dialog. When you have made all your selections click on **OK**.
3. Open the xml file from MS-Project®
Launch MS-Project and select **File ▸ Open** from the main menu. Change the file type to be 'XML Format (*.xml)' and choose the xml file from the list. From the import dialog that will appear you can either import the xml file as new project, append to the active project or merge the data into the active project. After you have selected the way you want to import the data click on OK to display the project data in the gantt chart.

14.2d Exporting Scheduling & Resource Consumption Data to SchedulePro

For users who need to combine scheduling and resource consumption data from several recipes as they all may execute in the same facility, or for those users who may still deal with a single recipe but when planning a campaign of multiple batches they would like to have a more refined control over the scheduling of each batch (and each operation in a batch), using SchedulePro (the companion software to SuperPro Designer in Intelligen's suite) is strongly preferred over MS-Project®. SchedulePro's utilities are much more tuned to engineers in process modeling and operations and make it much easier to analyze and debottleneck multi-product (and/or multi-batch) facilities.

▶ To export scheduling and resource consumption data to SchedulePro...

1. Select the **File ▸ Export to SchedulePro's Recipe DB** command from main menu of the application. The following dialog (Figure 14.3) will appear.

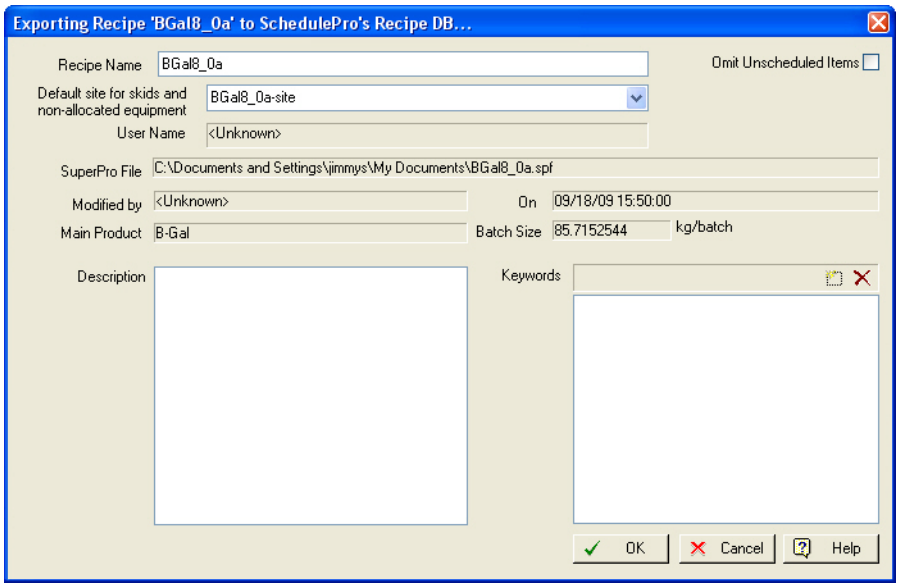


Figure 14.3:The 'Export to SchedulePro 's Recipe DB' dialog.

2. Fill in the data of the Exporting Recipe to SchedulePro's Recipe DB Dialog.
   You need to specify a name for the recipe and specify a site to be used as the assumed site for all sections that do not have an allocated site already. Even though not required, it is strongly recommended that you add a short description for the recipe and provide several appropriately selected keywords to be associated with this recipe so that it can be easily retrieved later if needed. come up. The Password For DB Access Dialog may precede the exporting dialog if the 'Always Show Password Dialog' option has been set in the Application Settings Dialog: Miscellaneous tab in the Database Access section.
3. Click on **OK** to start the exporting process.
   This may take several seconds or minutes depending on the size of your recipe. Sometimes, after click on **OK**, you may get the following message: *"You already have a recipe with that name in the database. Update it?"*. This message will come up if the there are already data recorded under the recipe name that you provided.

*If the **File ▸ Export to SchedulePro's Recipe DB** command is not available (greyed out) make sure you have SchedulePro currently installed on your PC. If not, please install SchedulePro first and then restart the process of exporting the data from SuperPro Designer to SchedulePro's Recipe DB. The actual database file behind the database source is "SP RecipeDBv6.mdb". Make sure that this file exists under the installation path for SchedulePro.*

14.3 EXPORTING / LINKING TABLES (GRIDS) TO MS-EXCEL

Several interfaces in SuperPro Designer present process data in the form of a grid:

- the Equipment Contents Dialog presents the contents of equipment with mass holding ability during the span of one or more procedures;
- the Procedure Activity Overview Dialog presents in a grid an overview of all the actions scheduled to execute inside a procedure's queue;
- the The Stream Summary Table is a highly customizable grid with information on a user-selectable set of streams that may be key to the process;
- the Registered Components Property Table presents all the key properties for the registered components in the process.

From all of the above grid interfaces, users have the ability to map (and link) the information presented within the application to an area in a MS-Excel spreadsheet. The procedure for accomplishing this is the same from all such interfaces.

▶ To Export/Link a table (grid) to MS-Excel® spreadsheet...

1. Present the table using the application's interface command.
   For example, to present the equipment contents of a vessel, select **Equipment Data** from the procedure's command (context) menu.
2. Once the grid is in display, select **Excel Link ▸ Edit** from the interface's command (context) menu, see Figure 14.4 (actual contents of the menu depend on the interface and may be slightly different than what shown inFigure 14.4). The command menu will be presented when you right-click over the grid.

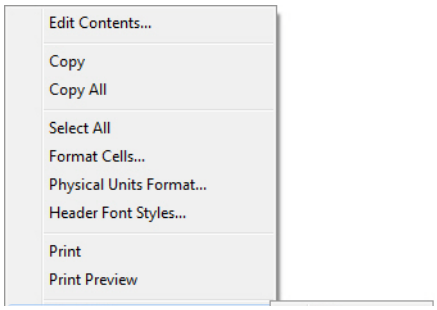


Figure 14.4:Customizing the Excel Link to a grid starts with accessing the grid's command menu.

3. The Link Table to MS-Excel® Dialog will appear. From there you can specify:
   - the 'xls' file (book) to be used as the container for the data.
   - the area (sheet and cell range) where the data will be deposited.
   - schedule when you wish to have the data updated.
   For more details on the above specifications, see Link Table to MS-Excel® Dialog.

If you have chosen to have the data updated automatically ('Auto-Update' option in the Link Table to MS-Excel® Dialog), then as soon as the data in the dialog change (e.g. due to M&E

balance execution) the corresponding area in the selected Excel book will also be updated as well. If you have chosen to have the data updated manually, then simply right-click and present the interface's context menu and then select **Excel Link ▸ Update**.

*All the properties of the grid-to-Excel link can be accessed by the COM engine of the application. Therefore users can customize the content and target area of such information transfer programatically (from a COM client environment). Furthermore, the activation of the data transfer (the equivalent of selecting **Excel Link ▸ Update** from the interface's command menu) is also an available COM command.*

When you no longer need to have the information linked (or transferred) to a MS-Excel book, you should delete the link (select **Excel Link ▸ Delete** from the interface's command menu).

14.4 IMPORTING OLE OBJECTS

SuperPro Designer not only makes it easy to share drawings and data with other programs, but also allows you to import foreign documents (such as MS-Word® files or bitmaps) or document fragments (portions of a MS-Excel® book) and make them part of your process file. Using Windows®' OLE (Object Linking and Embedding) technology, you can import an object copied into the clipboard from another OLE-server application (e.g., MS-Excel®, Corel Draw®, MS-Word®, etc.). For instance, let us assume that you have been working on some side calculations with MS-Excel® (related with a particular aspect of your process) and you would like to display them on your process flowsheet. You can copy and paste (or even better, paste-link) that portion of your book right into your process flowsheet. Here's how:

▶ To Import an OLE object into the process flowsheet...

1. Copy the original item
   Go to the application that created the OLE object, (e.g. MS Excel®) and copy the object (spreadsheet area) that you wish to display in the process flowsheet. Typically, selecting the object and then **File ▸ Copy** from the main menu (or **Ctrl+C**) would do it.
2. Click on an empty area of your flowsheet
   Before importing the object, you need to indicate to the program, where you wish to have the object pasted. You can do that by simply clicking on an unoccupied area of your process flowsheet. Make sure that you do not click over another element of your flowsheet, and that there is enough unoccupied space around the location to accommodate the size of your imported item. The application will place the imported item centered around the location of your last click.
3. Paste the object
   If you select **File ▸ Copy** or (**Ctrl+C**) the application will paste a copy of your OLE object into the flowsheet. If you select **File ▸ Copy Special,** then the dialog shown in Figure 14.5 will be shown. From that dialog you can either opt to:
   (a) Paste, or
   (b) Paste-Link
   the object. Paste-linking the object, establishes a hot-link between the original object (e.g. spreadsheet) and the displayed grid on your process flowsheet. Whenever the related

content changes, then the displayed information on your flowsheet will change too. If you chose to simply paste the object, then a frozen image of the object (as it exists now) will be pasted in your flowsheet and it will never be updated (even if the original object is modified).

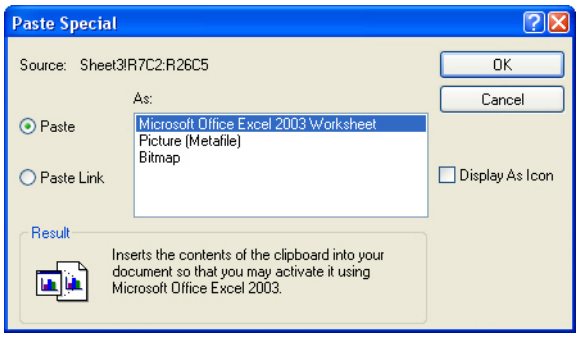


Figure 14.5:The 'Paste Special' dialog.

You can also initiate the creation of a new OLE object straight from your process flowsheet. In other words, you don't have to ever leave SuperPro Designer to initiate the creation of another object and have it pasted right there.

▶To insert a new OLE object in the process flowsheet...

1. Select **Edit ▸ Insert Object**
   Notice how the cursor changes to:

2. Click on an unoccupied area of your flowsheet
   Before creating the object, you need to indicate to the program, where you wish to have the object pasted. You can do that by simply clicking somewhere in your flowsheet. Make sure that you do not click over another element of your flowsheet, and that there is enough unoccupied space around the location to accommodate the size of your imported item. The application will place the imported item centered around the location of your last click.
3. Select object type
   A dialog similar to what is shown in Figure 14.6 will appear. Select the object type that you wish to create (spreadsheet, equation, etc.). The list of objects presented depends on the OLE servers registered in your Windows® environment.

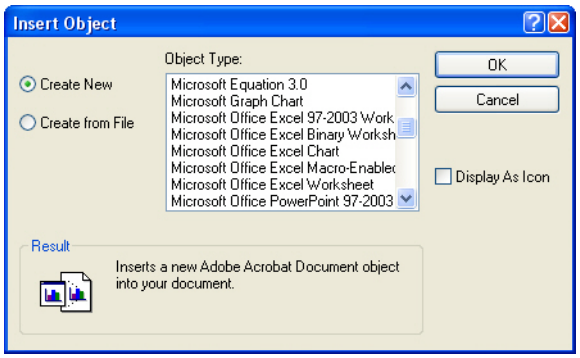


Figure 14.6:The 'Insert Object' dialog.

4. Click **OK**. Notice that the menus of the application have changed. They have been replaced by the menus of the server application that will selected in the 'Insert Object' dialog.

When a saved process (.spf) file that contains foreign OLE objects is opened in SuperPro Designer, the application will attempt to connect to each of the objects' server applications in order to properly display them. Therefore it is important that the next time you (or any of your colleagues that may be viewing this file) open it, you must have a compatible version of the server applications that created those objects. If you don't, an error message will be displayed during the opening of the file. If you intend to send the process file to a colleague that you know doesn't have access to embedded OLE objects in your file, you may save a version of your file without the objects (select ***File ▸ Save in a File without OLE Objects*** *from the main menu) and send him that file.*

14.5 USING SUPERPRO DESIGNER'S OLE SERVER

Using the Component Object Module (COM) technology, applications running under MS-Windows® can exchange information and services with each other once they register themselves as Object Linking and Embedding (OLE) Automation Servers. SuperPro Designer's installation script indeed registers SuperPro Designer as an OLE Automation Server. There are several applications that either themselves are a programming environment that provides COM client services (such as MS-Visual C++, MS-Visual C#, MS-Visual Basic, etc.) or they support a scripting language with utilities that can tap into COM client services (such scripting language in MS-Excel, MS-Word, etc.) The 'Designer' Type Library (and all its functions) is registered by SuperPro and EnviroPro Designer. It includes a long list of functions that can be used to accomplish various tasks, including (but not limited to): The Designer COM Server can thus be used by client applications to perform various tasks including:

- Starting or ending SuperPro Designer application; opening and closing process files.
- For an open process file, solve the M&E balances and perform the economic calculations.

- Fetch or set values to almost all data contained in a process file: input stream flows, compositions, etc, operating parameters for unit operations and/or unit procedures, sizes in equipment resources, etc.
- Generate reports, charts, etc. and export them to the clipboard (for later pasting in another application) or to 'wmf' files that can later be imported by another application.
- Retrieve error messages.

The extend of services provided by the 'Designer' type library is not meant to be a substitute for the entire user-interface of SuperPro Designer. For instance, users of the library cannot create (synthesize) a process using library calls; they can only load a pre-existing process file and parametrically (but not structurally) modify it. Therefore all the services are designed to deal with an existing process, already described and contained in a 'spf' file. As such it can be of great use for user who wish to:

(a) Transfer between applications and/or databases.

(b) Perform parametric studies for sensitivity analysis, process optimization, process economic evaluation, etc.

(c) Integrate SuperPro Designer with stochastic risks analysis tools in order to carry out risk assessment studies and stochastic modeling.

(d) Create custom reports for design, economic evaluation, and environmental assessment purposes.

Detailed documentation on how to use the SuperPro Designer's COM library module can be found in Appendix E (COM Library). The appendix is only part of the PDF version of the manual; it can also be viewed as part of the online help documentation when selecting **Help ▸ COM Interface & Library** from the main menu of the application.

15

DATABASES & DATABANKS

There are several types of entities (objects) that participate in a typical process simulation: materials (components and mixtures), utilities (heat transfer agents, power), consumables, etc. Many of these entities have constant properties and it would be very tedious to have to specify them every time you engage them in a new simulation project. SuperPro Designer supports the use of databanks to alleviate users from this burden. A databank is simply a collection of property descriptions for a set of similar objects stored away in a database file. SuperPro Designer allows users to populate databanks for pure components, stock mixtures, heat transfer agents, etc. so that their members can be easily retrieved and used by future projects. SuperPro Designer's databanks are collectively kept in database files in MS-Access® format. Each databank can be populated from the interfaces of the application or by opening the database file directly from MS-Access®. There are five such different database files that SuperPro Designer currently can use to store and/or retrieve data:

- The 'Designer' database (sometimes referred to as 'System' database)
- The 'User' database
- The 'Process' database
- The 'DIPPR' database, and
- The 'PPDS' & 'PPDS BIP' databases

The 'Designer', 'User', 'Process' and 'DIPPR' databases are registered as named 'Data Sources' with your operating system automatically during program installation. Each data source is assigned a database file to use as the repository and source for the data. All such database files are kept in a location that defaults to a 'DBases' folder under the auxiliary folder that is selected during installation (but can be customized during installation or later). A demonstration version of the DIPPR databank with only 5 components is one of the files copied in that directory. If the full DIPPR database file is already at the user's disposal or if it becomes available after installation, it has to be reported to SuperPro Designer in order for the application to start taking advantage of its contents. The 'PPDS' database type files can only be used if the user has a licensed copy of the PPDS Thermodynamic Property Suite from TUV SUD installed on his or her system. For information on how to assign a new database file to one of the five data sources used by the application, see 15.1 Database Registration.

The 'Designer' or 'System' database is maintained and constantly updated (from release to release) by our staff at Intelligen and its contents cannot be edited by the end user. The 'User' database, at the time of installation, does not contain any actual data, only empty databanks (aka relations or tables) that can be later filled in by the user. The 'User' database exists to receive from end users descriptions of entities like pure components, heat transfer agents, labor types, consumables, processing sites etc. according to their needs. The 'DIPPR' database file contains only one databank for pure components. It has been developed and maintained at

Brigham Young University. When the time comes to introduce (register) a pure component into your process, the 'DIPPR' database will appear as a database source option in the Pure Component Registration Dialog. The 'PPDS' database files supported by SuperPro Designer are the Pure Component and the Binary Interaction Properties databank files in MS-Access format. Pure components from the 'PPDS' database can be registered in the process in the same way as components are from the 'DIPPR' database (simply change the 'source' databank). Binary Interaction Property coefficient values are imported automatically upon registration of the pure components of the binary mixture, if no other binary coefficient can be found for that pure component pair in the 'System' or the 'User' databases.

The 'Designer' and 'User' databases hold in their contents the following databanks:

- Pure Components
- Stock Mixtures
- Binary Coefficients
- Heat Transfer Agents
- Power Types
- Labor Types
- Consumables
- Equipment Materials
- Currencies
- Sites & Site Resources (Equipment, Labor Types, Heat Transfer Agents, Power Types)
- Vendor-Equipment
- Vendors/Manufacturers
- Equipment Type Specifications
- Specification Variables
- User Defined Equipment Purchase Cost Models

When users modify an object's property as kept in its 'User' databank (e.g. a stock mixture's price), this change does not automatically propagate to all process files that may be using this object. Similarly, for users who take advantage of database site objects and their resources (see 'Section Allocation' on page 8-6, and 6.1i Equipment Allocation) it does not imply that when the database object's properties change, it automatically affects the properties of the corresponding object in a pre-existing process file. Instead, the program has several interfaces that allow you to update the values of database objects contained in process simulation files based on the latest information in the database, but this process must be initiated by the user. This is done intentionally in order to protect existing process files from changes in database files that users may not wish to have propagated to their own projects.

For users with files that contain allocations to database sites or any of their resources (see Sites & Resources Databank), the application will check for consistency between the objects as contained in a process file and their database counterparts if you select **File ▸ Check Consistency with Site DB** from the main menu. The ensuing Reconcile with Site DB Dialog informs the user about any inconsistencies that may exist.

For users with files that engaged entities from the 'User' database (such as Pure Components, Stock Mixtures, Labor Types, Heat Transfer Agents, etc.) but without explicit section allocation to database sites, they can still bring up the corresponding entities registry (aka 'Currently-in-Use') dialog and from there they can selectively update any objects in their files based on the database's counterpart, or reversely, update the database's object based on the property values as they exist in the file. For example, if you select **Tasks ▸ Other Resources ▸ Heat Transfer Agents** from the application's main menu, you can bring up the List of Heat Transfer Agents Currently in Use. From there, you can select a specific agent and either update its properties based on the current values in the databank (using the button) or request that the databank's corresponding object is updated using the values as they exist in the current file (using the button).

The Processes Databank contains information about completed processes (their unit procedures, operations, consumables, etc.) in a MS-Access® (searchable) format. For each process record, the databank also maintains a set of keywords. The Processes Databank can be used to compile a catalog of completed projects so that they can be easily searched later (based on their contents, keywords, etc.).

To avoid unintentional access to data, all database files are password-protected (see 'Database Passwords' on page 15-4). The 'Designer' database password can be provided upon request to users interested in expanding or modifying the database using MS-Access® directly (bypassing the interfaces of SuperPro Designer) or for users who would want to access the data from other applications (by code). For typical use, it is highly recommended that the databases (and the databanks contained therein) be updated and maintained from the interfaces that SuperPro Designer provides. All these interfaces can be accessed through the **Databanks** menu.

15.1 DATABASE REGISTRATION

Upon installation, SuperPro Designer automatically registers four of the databases with the operating system as named data sources and makes them immediately available to the application. Each data source is assigned to use its own file. All files are password-protected and they are originally (by installation) located in the same folder ('DBases' under the auxiliary installation directory). If the database files are moved to another location or their file name is modified or the password is changed or an alternative database file is to be used, you should inform the program accordingly. You should also inform the application if you have purchased (or have at your disposal already) the full DIPPR database file. Furthermore, if you have a licensed version of the PPDS Suite of applications you may also register the Pure Component and/or the Binary Interaction Property 'PPDS' databases. To accomplish any of that, select **Databanks ▸ Availability, Passwords, & Locations** from the main menu and provide the new information in the Databases: Availability, Password & Locations Dialog that appears. It is the responsibility of the users to make sure that the password recorded within the application matches exactly the password of the corresponding database files. Otherwise, the application will not be allowed to open and modify databanks contained in the files.

DATABASE PASSWORDS

The database (MS-Access®) files supplied with the program are all protected with a password:

for Designer (or System) Database	Please contact Intelligen, Inc. if needed
for User Database	"changeme"
for Process Database	"changeme"
For DIPPR DB	Unknown

Every time the application accesses any of the above files, it needs to use the correct password. All of the above files can be opened directly from MS-Access® 2000 (or later). Since we do not assume that you should modify the 'Designer' or the 'DIPPR' database, their passwords are not revealed. You should receive the password protecting the 'DIPPR' database once you have purchased the full version. The only other file that you may want to modify from the MS-Access® development environment (or using a third-party utility) is the 'User' database file (and for that the password is supplied, see above).

If you open the 'User' file with MS-Access® and change the file's password, you will have to inform the application about the new password, otherwise SuperPro Designer will not be able to open the file and access its contained databanks when needed. For example, when attempting to register a pure component that you know it exists in the 'User' databank, SuperPro Designer will be denied access to fetch its properties. The same holds true for the 'DIPPR' (full version) relational database. You must visit the Databases: Availability, Password & Locations Dialog and from there the Update Database Password Dialog to inform the application about the new passwords. A password may be provided even for the 'PPDS' databanks if those database files are password protected.

CHANGING A PASSWORD FROM MS-ACCESS®

If you wish to remove or change the password of the 'User' database, you must first open the database (with exclusive rights) in MS Access®. Start then MS-Access® interface and then select the **File ▸ Open** menu option. After locating the database file in the file selection dialog, select the option **Open Exclusive** in the combo box located in the bottom-right corner of the dialog. After providing the current password and gaining access to the database, select **Security** from the **Tools** pull-down menu, and then **Unset Database Password**. You will be prompted to enter the current password. The current password will then be removed. After this is done and if you wish to set a new password, select again **Security**, then the option **Set Database Password** and provide the new password. For MS-Access® 2007 users open the file in the same way exclusively and from the ribbon bar visit the **Database Tools** tab and select

the **Unset Database Password** icon button to unset the existing password or **Set Database Password** to set a new password.

In order for SuperPro Designer to be able to access the databases at run-time, it needs to be informed about the updated passwords. To do that, run SuperPro Designer and select ***Databanks ▸ Availability, Password & Locations****. In the Databases: Availability, Password & Locations Dialog that opens, press the* ***Password*** *button in the affected database section and provide the new password. If the password of the database has been removed (i.e. the database is no longer password protected), leave the password box blank and click* ***OK****. Note that changing the password through SuperPro Designer alone, does not automatically change the password of the database file itself. You have to go through MS-Access following the process described above.*

15.2 IMPORTING DATA FROM ANOTHER 'USER' DATABASE

It is possible that more than one users in the same company or institute that runs the application may have created their own 'User' databases and populate them with their own customized resources (components, heat transfer agents, consumables, equipment, etc). Sometimes corporate users may create several 'User' databases, depending on their location. These users may want to have access to each other's data or possibly even combine their data and create one common 'User' database which should become available on a shared location on the network (perhaps with different access privileges for each user). Before this happens, you may want to import data from one database file to another.

Please note that this process will import (selectively) the following databanks:

- Pure Components
- Stock Mixtures
- Binary Coefficients
- Heat Transfer Agents
- Power Types
- Labor Types
- Consumables
- Equipment Construction Materials
- Equipment Specification Variables
- Currencies
- Equipment User Defined Cost Models

However, the import procedure, *will not be able* to import the following databanks:

- Sites
- Equipment in Sites (or Site-Equipment)
- Vendor-Equipment (Equipment Spec Sheets)
- Vendors/Manufacturers
- Equipment Types & Specifications

Importing data from another database's databank requires that the source databank is located in a database file that came pre-formatted with SuperPro Designer. The source databank cannot be in another vendor's database file. Also, the import process requires that both source and destination database files are of the same version. If the source databank is of an older format, then you must upgrade it (or better yet upgrade a copy of it) using the **Databanks ▸ Upgrade a Past Version User DB File...** option from the main menu, then use the converted file as a source for import. The actual copying of the data is done using the Import Database Data Dialog that appears when you select **Databanks ▸ Import Data into the Active User DB** from the application's main menu.

15.3 ACCESSING DATA IN OLDER 'USER' DATABASES

When upgrading to a new version of the software the databanks contained in the 'System' and 'User' database files most probably have been upgraded as well. You know that the database's version has changed if the file name has changed. If you have populated your 'User' databanks with lots of entries (components, mixtures, sites, equipment, vendors, etc.) chances are you need to gain access to that data from your new SuperPro Designer version. You can gain access to the data contained in your old 'User' database file by adopting one of the following two options:

A. UPGRADING ALL 'USER' DATABASE CONTENT...

If you want to make the entire contents of the previous 'User' database file available to the new version, then the process is very simple. First make a copy of the previous 'User' database file (for backup purposes). Then, simply use the Databases: Availability, Password & Locations Dialog and force the newest version of SuperPro Designer to use the old 'User' database file. That's it. The file will be automatically converted to the latest format and all the contained databanks will be available for immediate use in your future projects. It is recommended that you change the name of the new database file in a way that is reminiscent of its version number in order not be confused in the future with the file used by the previous version.

B. UPGRADING SELECTED 'USER' DATABASE CONTENT...

If you want to make only portions of the data in the old 'User' database file available to the new version of SuperPro Designer, then you should use the Import Database Data Dialog (see 15.2 Importing Data from Another 'User' Database). Please note that data importing is a very sensitive process that could fail if it creates conflicts with data preexisting in the databank, e.g. if it attempts to import a component that already exists in the new databank. Users are warned for such conflicts and if the number of failures exceeds a limit, the transfer process is aborted. Therefore, it is highly recommended that this process be executed when the destination 'User' database is still fairly empty (ideally, right after installation of a new release of SuperPro Designer). Some entities (e.g. site descriptions including their resources such as labor types, heat transfer agents, etc.) cannot be imported currently with this method. For this reason or if

you have extensive data in the above databanks, it is recommended that you upgrade the entire 'User' database file (option (a) above).

Before up-converting any old database files, it is highly recommended that you keep a backup copy of the file as once it is converted it can no longer be used by the old version of the software. Also, make sure that you have write privileges to the source user database and that the file is not write protected. If it is password protected, then verify that you have the current password.

15.4 PURE COMPONENTS DATABANK

Chemical components are used to represent the flow and composition of material in streams. They are also used as ingredients in stock mixtures (see 15.5 Databank of Stock Mixtures) to initialize flows of input streams. Pure components can also serve as special-purpose agents in some operations (CIP, Gas Sweep, etc.). The pure components databank included in the 'Designer' (or 'System') database includes over 500 components and it is occasionally updated by our staff. SuperPro Designer also supports the DIPPR pure components databank in its relational database form, as developed and maintained at Brigham Young University. The DIPPR databank contains over 1700 pure components along with their physical and thermodynamic properties compiled from literature. Starting with version 9.5, SuperPro Designer can also access pure component property data from the PPDS database format available from TUV SUD.

It should be made very clear that purchasing a license to SuperPro Designer does NOT include purchasing the rights to own and use the PPDS database. Intelligen, Inc. merely provides the means to import data from a PPDS database, provided that the owner of SuperPro Designer has purchased and maintains an active license for the use of PPDS databases.

15.4a Viewing the Contents of the Pure Components Databank

To access the components databank, use the **Databanks ▸ Pure Components** menu item from the main menu (or hit **F2** as a shortcut). The ensuing Pure Components Databank Dialog displays a list of all the pure components that exist in the 'Designer' and 'User' databases. The pure components available in the 'DIPPR' or the 'PPDS' database, can be shown by clicking on the 'Database Filter..' button and selecting the 'DIPPR' or the 'PPDS' option respectively.

If you select a pure component that belongs to the 'Designer', 'DIPPR' or the 'PPDS' database you can only view (but cannot modify) the contents of that databank. Clicking on the button will present the Pure Component Properties Dialog (in view-only mode). If you choose a pure component that resides in the 'User' database, then you will be able to view as well as modify the properties of the members in that components databank. Clicking on the button will present the same Pure Component Properties Dialog but this time, you can view as well as edit (and save) the properties of the selected component. Finally you may also add a new component or delete existing component descriptions from the 'User' database (see 15.4b Adding and Deleting Pure Components).

15.4b Adding and Deleting Pure Components

In order to add a new component, bring up the Pure Components Databank Dialog by selecting **Databanks ▸ Pure Components** from the main menu of the application. When adding a new pure component, it will be saved by default in the 'User' database. Keeping the newly introduced component in the 'User' databank will make it readily available for use in any future process simulations. Click on the button and fill up the fields in the New Component Definition Dialog. After you exit the dialog by clicking on **OK**, and if the suggested names are accepted, a new entry will be created in the table of contents representing the new component. The new component's formal name must be unique amongst all components in the 'User' databank. It is allowed to introduce a component with the same formal name as another component in the 'Designer' databank. The new component will first be created with property values that are copies of a pre-existing component, but it can later be customized to match your specifications. Select the line representing the newly created component and then click on the button to bring up the Pure Component Properties Dialog in order to adjust the component's property values. If you wish to delete a component from the 'User' databank, select the line in the table of contents that represents the component and then click on the button.

Deleting a component from your 'User' components databank does not affect any existing process files that may have utilized (registered) this component. All previous projects utilizing this component already contain a complete definition of every component engaged in that simulation inside their document (file) and do not depend on the continued presence of such components in the databanks ('User', 'Designer', 'DIPPR' or 'PPDS') in order to continue to produce simulation results.

15.5 DATABANK OF STOCK MIXTURES

Stock mixtures accelerate the initialization of feed streams in cases where some raw material (e.g., a buffer, a caustic solution, etc.) is used 'as-is' and it is a mixture of pure components and possibly other stock mixtures. The 'Designer' portion of the databank includes the definition of over 40 mixtures that can be readily registered in a process simulation. Users can introduce their own descriptions of stock mixtures in the 'User' portion of the databank to extend the list.

15.5a Viewing the Contents of the Stock Mixtures Databank

To access the stock mixtures databank, select the **Databanks ▸ Stock Mixtures** menu item from the main menu (or hit **Shift+F2** as a shortcut). In the Stock Mixtures Databank Dialog that comes up, you will see a list of all the stock mixtures that exist in the 'Designer' and the 'User' database. Using the 'Database Filter..' button you may choose to display the contents of either source or both.

If you select a stock mixture that resides in the 'Designer' database you can only view (but cannot modify) its properties (and of course, you cannot delete the mixture). Clicking on the button will present the Stock Mixture Properties Dialog (in view-only mode) where you can inspect all of the mixture's properties. If you choose a stock mixture that resides in the 'User' database, then you will be able to view as well as modify its properties. Clicking on the button will present the same Stock Mixture Properties Dialog but this time, you can view as well as edit (and save) the properties of the selected mixture. You may also choose to delete

an existing mixture and/or add a new mixture using as a basis other components and/or mixtures currently residing in your component and/or mixture databanks (see 15.5b Adding and Deleting Stock Mixtures).

15.5b Adding and Deleting Stock Mixtures

A new stock mixture can be added to the databank kept in the 'User' database. The new stock mixture will first be created to have property values that are copies of a pre-existing mixture, but it can later be customized to match your specifications. Keeping the newly introduced mixture in the databank ('User' portion) will make it readily available for use in any future process simulations. In order to add a new mixture, bring up the Stock Mixtures Databank Dialog by selecting **Databanks ▸ Stock Mixtures** from the main menu of the application. On this dialog, click on the button and fill up the fields in the New Stock Mixture Definition Dialog. Then click on the button to bring up the Stock Mixture Properties Dialog in order to adjust the mixtures properties. In order to delete a mixture from the 'User' database, select the line in the table that represents the mixture that you wish to delete and then click on the button..

Deleting a stock mixture from your mixture databank does not affect any existing process files that may have utilized (registered) this mixture. All previous projects utilizing this mixture already contain a complete definition of every mixture engaged in that simulation inside their document (file) and do not depend on the continued presence of such mixtures in the databanks ('User' or 'Designer' portion) in order to continue to produce simulation results.

15.6 BINARY COEFFICIENTS DATABANK

Binary coefficients are used in several thermodynamic models (e.g. equations of state or activity coefficient models) in an attempt to capture non-ideal behavior of mixtures. The 'Designer' database includes binary coefficients for over 60 binary mixtures. More will be added in future releases. Starting with version 9.5, SuperPro Designer provides the support for accessing binary coefficients from the 'PPDS' Binary Interaction Property databank, which is available in the PPDS Thermodynamic Property Suite application from TUV SUD.

It should be made very clear that purchasing a license to SuperPro Designer does NOT include purchasing the rights to own and use the PPDS database. Intelligen, Inc. merely provides the means to import data from a PPDS database, provided that the owner of SuperPro Designer has purchased and maintains an active license for the use of PPDS databases.

For more information on the binary coefficients and the thermodynamic models that use them, see 3.1i Component Properties in a Binary Mixture and Vapor-Liquid Equilibrium Modeling.

15.6a Viewing the Contents of the Binary Coefficients Databank

To access the binary coefficients databanks, select the **Databanks ▸ Binary Coefficients** menu item from the main menu. In the Binary Coefficients Databank Dialog that appears, you can see a list of all the available binary coefficients in the 'Designer, the 'User' and the 'PPDS' database if available. If you select a binary mixture that resides in the 'Designer'or the 'PPDs' database then you can only view (but not modify) the binary coefficients, whereas if you select

a binary mixture that belongs to the 'User' database then you will be able to view as well as modify the values of binary coefficients in the databank. Using the 'Database Filter..' button you may choose to display only the 'Designer', 'User' or the 'PPDS' database binary mixtures. Finally you can also add new binary mixtures by selecting two Pure Components from the 'Designer', 'User' or 'DIPPR' pure component databanks and adding them to the list of existing binary mixtures. Binary coefficient values can then be added manually or by copying existing values from other binary mixtures.

15.6b Adding and Deleting Binary Coefficients

A new binary coefficient for one or more thermodynamic models can be added to the databank kept in the 'User' database. Keeping the newly introduced binary coefficient in the 'User' databank will make it readily available for use in any future process simulations. In order to add a new binary coefficient, bring up the Binary Coefficients Databank Dialog by selecting **Databanks ▸ Binary Coefficients** from the main menu of the application. On this dialog, choose the two components (i,j) for which you wish to introduce a new binary coefficient (b_{ij}). You may choose two different pure components from either the 'Designer', the 'User' or the 'DIPPR' databases. Finally click on the button to add the new binary mixture to the table on the left, and edit the coefficients for this mixture. Binary coefficient values may be also copied from another binary mixture by selecting the mixture and then clicking on the copy button . Then select the binary mixture you wish to copy the values to and click on the paste button . In order to delete a pre-existing set of binary coefficients for a pair of components (i,j), you must first select the component pair (binary) as shown in the table listing and then click on the button.

15.7 HEAT TRANSFER AGENTS DATABANK

Heat transfer agents are used by SuperPro Designer in many operation types either directly or indirectly. Direct use implies that the operation's simulation model can account for one (or more) heating or cooling duties as part of the expected function of the operation. The heating or cooling requirements typically are presented on the 'Oper. Cond's' tab of the i/o simulation dialog. The application expects the user to choose an appropriate agent that is assumed to carry out the heating/cooling assignment. Besides the direct use, heat transfer agents may be engaged to carry out auxiliary heating/cooling loads (indirect use). Such loads can be associated with any operation (regardless of its model) and they can be specified from the Operations Dialog: Labor, etc Tab. Each heat transfer agent carries along several parameters (supply & return temperatures, mass-to-energy factor, cost, etc.); for more details, see 6.7d Heat Transfer Agent Properties. The application comes with a small set of preexisting agent definitions for heating (Steam, HP Steam, Brine, etc.) and cooling (Cooling Water, Chilled Water, etc.) These agents are part of the 'Designer' portion of the databank. However, users may add their own definitions by populating the 'User' portion of the databank.

15.7a Viewing the Contents of the Heat Transfer Agents Databanks

To access the heat transfer agents databanks, select the **Databanks ▸ Heat Transfer Agents** menu item from the main menu. In the Heat Transfer Agents Databank Dialog that will appear, you may see the full list of available heat transfer agents from the 'Designer' and the 'User'

databases. Using the 'Database Filter..' button you may choose to display only the 'Designer' or 'User' database agents.

If you select a heat transfer agent that belongs to the 'Designer' database you can only view (but cannot modify) its properties. Clicking on the button will present the Heat Transfer Agent Properties Dialog (in view-only mode) where you can inspect all of the agent's properties. If you choose a heat transfer agent that resides in the 'User' database, then you will be able to view as well as modify the properties of the members in the agent's databank. Clicking on the button will present the same Heat Transfer Agent Properties Dialog but this time, you can view as well as edit (and save) the properties of the selected agent. Finally you may also add a new definitions as well as delete any heat transfer agent definitions that you no longer need (see 15.7b Adding or Deleting a Heat Transfer Agent).

15.7b Adding or Deleting a Heat Transfer Agent

Before a previously undefined heat transfer agent can be used in a process simulation, it must be first introduced in the agent databank ('User' database). Keeping the newly created heat transfer agent in the agent databank will make it readily available for use in any future process simulations. To add a new heat transfer agent, bring up the Heat Transfer Agents Databank Dialog by selecting **Databanks ▸ Heat Transfer Agents** from the main menu of the application. On this dialog, click on the button and in the edit dialog type in the name of the new heat transfer agent. After you type in an acceptable name (must be unique amongst all heat transfer agents in the databank,) a new line will be added in the table to represent the new agent. Notice that all of the agent's properties have been assigned default values but of course they can be edited to their proper values (click on to present the Heat Transfer Agent Properties Dialog and specify the appropriate values for the properties of the new agent). If you want to delete a heat transfer agent from the databank, select the line in the table of contents that represents the agent that you wish to delete and then click on the button. Remember that you can only delete agents that reside in the 'User' portion of the databank.

Deleting a heat transfer agent from your databank does not affect any existing process files that may have utilized (registered) this agent. All previous projects utilizing this agent already contain a complete definition of every heat transfer agent engaged in that simulation inside their document (file) and do not depend on the continued presence of such agents in the databank ('User' or 'Designer' database) in order to continue to produce simulation results.

15.8 POWER TYPES DATABANK

Power may be required for the execution of several types of operations either directly or indirectly. Direct use of power is typically specified on the 'Oper. Cond's' tab of the i/o simulation dialog of the operation. Indirect use of power may be specified as auxiliary power and can be specified (for any operation) at the Operations Dialog: Labor, etc Tab. There are also some operations that generate power (see A.23 Power Generation Operations). As power may be available to plant locations from several suppliers (power networks) and therefore at different rates and availability limits, users may need to specify different power types and introduce them as needed in a process simulation. Each power type carries along several parameters (voltage, price, etc.); for more details on these parameters, see 6.9d Power Type

Properties. The power types databank is a repository where you can record power types that may typically appear in your simulations so that the can be shared in a consistent manner.

15.8a Viewing the Contents of the Power Types Databank

To access the power databanks, select the **Databanks ▸ Power Types** menu item from the main menu. In the Power Types Databank Dialog that comes up, you may see a list of all the available power types in the 'Designer' and the 'User' databases. Using the 'Database Filter..' button you may choose to display only the 'Designer' or 'User' database power types. If you select a power resource that belongs to the 'Designer' database you can only view (but cannot modify) its properties. Clicking on the button will present the Power Type Properties Dialog (in view-only mode) where you can inspect all of the power properties. If you choose a power resource that resides in the 'User' database, then you will be able to view as well as modify the values of any power type. Clicking on the button will present the same Power Type Properties Dialog but this time, you can view as well as edit (and save) the properties of the selected power resource. Finally you may also add new definitions as well as delete pre-existing power type definitions that you no longer need (see 15.8b Adding or Deleting a Power Type).

15.8b Adding or Deleting a Power Type

Before a previously undefined power type can be used in a process simulation, it must be introduced in the power type databank. Keeping the newly created power type in the databank will make it readily available for use in any future process simulations. To add a new power type, bring up the Power Types Databank Dialog by selecting **Databanks ▸ Power Types** from the main menu of the application. On this dialog and then click on the button and in the edit dialog that appears type in the name of the new power type. After you type in an acceptable name (must be unique amongst all power types in the databank,) a new line will be added in the table to represent the new power type. Notice that all of the power type properties have been assigned default values but of course they can be edited to their proper values (click on to present the Power Type Properties Dialog and specify the appropriate values for the properties of the new power). In order to delete a power type from the databank, select the line in the table that represents the power type that you wish to delete and then click on the button. Remember that you can only delete power types residing in the 'User' database only.

Deleting a power type from your databank does not affect any existing process files that may have utilized (registered) this power. All previous projects utilizing this power already contain a complete definition of every power type engaged in that simulation inside their document (file) and do not depend on the continued presence of such power types in the databank ('User' or 'Designer' portion) in order to continue to produce simulation results.

15.9 LABOR TYPES DATABANK

Every operation can be assigned several labor engagements. For each engagement the user must select a labor type (or a specific staff member) and a labor rate (how many labor hour / operation hour needed). The labor specifications for each operation are done in the Operations Dialog: Labor, etc Tab. Sections can also assume one or more labor overhead assignments (specified in the Operating Cost Adjustments Dialog: Labor Tab). Each labor type (or staff

member) is characterized by several parameters (basic rate, benefits factor, etc.); for more details, see 6.11d Labor Type Properties.

15.9a Viewing the Contents of the Labor Types Databank

To access the labor databanks, select the **Databanks ▸ Labor Type** menu item from the main menu (or hit **Shift+F3** as a shortcut). In the Labor Types Databank Dialog that will appear, you may see a list of all the available labor types that exist in the 'Designer' and the 'User' databses. Using the 'Database Filter..' button you may choose to display only the 'Designer' or the 'User' database labo types.

If you select a labor type that belongs to the 'Designer' database you can only view (but cannot modify) the properties of this labor. Clicking on the button will present the Labor Type Properties Dialog (in view-only mode) where you can inspect all of the labor type's properties. If you choose a labor type that resides in the 'User' database, then you will be able to view as well as modify its properties. Clicking on the button will present the same Labor Type Properties Dialog but this time, you can view as well as edit (and save) the properties of the selected labor type. Finally you may also add a new definitions as well as delete any existing definitions of labor types that you no longer need (see 15.9b Adding or Deleting a Labor Type).

15.9b Adding or Deleting a Labor Type

Before a previously undefined labor type can be used in a process simulation, it must be introduced in the labor databank. Keeping the newly created labor type in the labor databank will make it readily available for use in any future process simulations. To add a new labor type, bring up the Labor Types Databank Dialog by selecting **Databanks ▸ Labor Type** from the main menu of the application. On this dialog click on the button and in the edit dialog that appears type in the name of the new labor type. After you type in an acceptable name (must be unique amongst all labor types in the labor type databank,) a new line will be added in the table to represent the new labor type. Notice that all of the labor type properties have been assigned default values but of course they can be edited to their proper values (click on to present the Labor Type Properties Dialog and do the editing). In order to delete a labor type from the databank, select the line in the table that represents the labor that you wish to delete and then click on the button. Remember that you can only delete labor types residing in the 'User' portion of the databank (with records in the 'User' database).

Deleting a labor type from your databank does not affect any existing process files that may have utilized this labor. All previous projects utilizing this labor already contain a complete definition of every labor type engaged in that simulation inside their document (file) and do not depend on the continued presence of such labor types in the databank ('User' or 'System' portion) in order to continue to produce simulation results.

Users have the ability to define specific staff members ("John Q.", "Jane M.", etc.) and assign them in places where labor is required. In other words, instead of simply selecting a labor type (e.g. 'QC Operator'), you may want to assign specifically "John Q." (who has been introduced in the database as a 'QC Operator'). Staff members are not introduced from the labor databank interface. Instead, they are introduced from the Sites & Resources Databank Dialog so that specific staff members are introduced as instances of a given labor type available only within a given site. In order to employ the services of a specific staff member, you must first allocate your sections to database sites (see 'Section Allocation' on page 8-6).

15.10 CONSUMABLES DATABANK

Some types of equipment require the use of a consumable. For example, chromatography columns require the use of some type of resin, some membrane filters require the use of disposable cartridges, etc. The program maintains a list of consumable categories such as filter cartridges, disposable bags, etc. For each category, there's also a preset list of actual consumable types (such as DF Cartridge, 10L bag, 5L bag, etc.) that can be assigned to equipment that either need to have it (as a **required consumable**) or that the user decides to associate their use with the operation of the equipment as they may represent a significant cost item (**optional consumable**), see 6.1h Consumables. New categories of consumables (and new members of pre-existing or user-defined categories) can be added in the consumables databank and used in association with the operation of any compatible equipment; the specification of consumables utilized by an equipment resource is done through the Equipment Data Dialog: Consumables Tab of that equipment. The description of all consumable categories and actual consumable types that are required by the use of equipment supported by the software are all included in the 'Designer' database. Any extra members of the pre-defined categories, or any new categories or actual consumables introduced by the user are kept as part of the 'User' database.

15.10a Viewing the Contents of the Consumables Databank

Unlike all previous entities, when viewing the list of available consumables (aka consumables databank) you do not need to specify the source databank ('Designer' or 'User'). When you select **Databanks ▸ Consumables** from the main menu, you will be presented with the Consumables Databank Dialog that shows the entire set (as kept in both databases) of available consumable categories on the left pane. When a given node (category) in the left pane is selected, then for that consumable category, the interface displays all its known members (consumables or consumable types) on the right pane. The icons representing consumable categories with records in the 'Designer' database appear in red to indicate that they cannot be deleted (or have their properties changed). The same color-coding applies to the actual consumables (or consumable types) shown on the right pane: those shown in red cannot be removed. This is done to make sure that for all equipment supported by the application that require the use of a consumable, there is at least one choice available to the user. Of course users can add more choices (consumables) as possible options for required consumables. Users can also add more consumable categories and members of their own user-defined consumable category. These definitions are kept in the 'User' database and can be modified or even deleted by the user. To view the properties of a consumable category, select its node (on the left pane of the Consumables Databank Dialog) and click either on the view or the view/edit button (for pre-existing or user-defined entries). You can also right-click on the node and select **Edit Category** or double-click on the node as a shortcut. Similar options exist for the consumable types of a selected category (as displayed in the right pane).

15.10b Adding and Deleting a Consumable Type (Category)

You can extend the list of pre-existing consumable categories by adding your own. After you bring up the Consumables Databank Dialog, you can either click on the add new button shown over the left pane, or select **Add New Category** from the right-click menu of the parent node for all types (labelled 'All Consumable Categories'). In the Consumable Category

Dialog that will appear you must describe the new consumable type and click **OK**. A new node will be added under the 'All Consumable Types' parent node. Notice that the node will be of green color to indicate that it represents a user-defined consumable type. Only user-defined consumable types can be deleted. To delete a user-defined consumable type, select it and click on the delete button shown over the left pane of the dialog.

15.10c Adding and Deleting a New Consumable

You can expand the list of options available under a pre-existing consumable category or under a user-defined category by adding your own members. Bring up the Consumables Databank Dialog and select the category for which you wish to introduce a new consumable. The existing members will be shown at the right pane. Now you can either click on the add new button shown over the right pane, or select **Add Consumable** from the right-click menu of the parent node for this type (shown as the head node on the right pane). In the Consumable Properties Dialog that will appear you must describe the new consumable and click **OK**. A new node will be added under the parent node of the selected consumable category. Notice that the node will be of green color to indicate that it represents a user-defined consumable. Only user-defined consumables can be deleted. To delete a user-defined consumable, select it and click on the delete button shown over the right pane of the dialog.

15.11 EQUIPMENT MATERIALS DATABANK

Materials of construction are used by SuperPro Designer as one of the possible adjustments to the estimation of their purchase cost, see 'Purchase Cost Adjustments' on page 6-9. Equipment that use the built-in purchase cost estimation model receive a cost estimate based on an assumed material of construction (the assumption is part of the built-in cost model) and later they use their actual material factor to adjust (scale) the final estimate. The 'Designer' database contains an equipment materials databank with a limited set of records for construction materials and only for some of the equipment types supported by the application. However, users may extend the list of material factors by populating the 'User' databank.

15.11a Viewing the Contents of the Equipment Materials Databank

To access the equipment materials databanks, use the **Databanks ▸ Equipment Materials** menu item from the main menu (or hit **Shift+F3** as a shortcut). In the Equipment Materials Databank Dialog that comes up you get a list of all the available materials that exist in the 'Designer' and the 'User' database. Using the 'Database Filter..' button you may choose to display only the 'Designer' or the 'User' database materials. If you select an equipment material that belongs to the 'Designer' database you can only view (but cannot modify) the material factor (notice that the button over the table is inactive). However if you select a material that has no material factor specified (they are shown in pink color and have -1.0 as their value) you may edit its material factor even if the material itself only exists in the 'Designer' database. If you choose an equipment material that resides in the 'User' database, then you will be able to view as well as edit its material factor or even delete it (see 15.11b Adding and Deleting Equipment Materials).

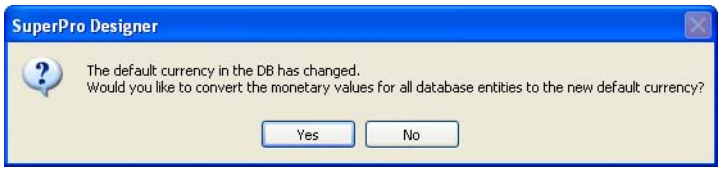
15.11b Adding and Deleting Equipment Materials

A new material can be added to the databank kept in the 'User' database. Keeping the material in the 'User' databank will make the corresponding material factor for an equipment type readily available (as an option) in any future process simulations that may use that equipment resource. In order to add a new material, bring up the Equipment Materials Databank Dialog by selecting **Databanks ▸ Equipment Materials** from the main menu of the application. The table below will show all the materials and their factors that are currently defined in the databank for the selected equipment type. To edit the material factor for an existing entry, simply click in the cell of the value and edit the factor. If you want to introduce a new material, click on the button and type the name for the new material. Please note that the material name must not conflict with any other materials already defined in the 'User' or the 'Designer' databank. After the name is accepted, a new entry will be added in the table and be given the default value of '-1'. Click in the cell of the factor and type the correct value. If you wish to delete a material, select the line representing the factor you wish to delete from the table by clicking on the row button (showing the index of the entry) and then click on the button.

Deleting a material from the 'User' materials databank or changing its material factor value does not affect any existing process files that may have utilized the corresponding material factor. All previous projects utilizing this material already contain a copy of that factor and they do not depend on the continued presence of such factors in the databanks ('User' or 'Designer') in order to continue to produce simulation results.

15.12 CURRENCIES DATABANK

For all our international users, SuperPro Designer allows you to input cost items, prices and view economic reports in your own local currency. Since all built-in equipment purchase cost estimators produce figures in US$, SuperPro Designer will need to convert the estimated prices to your currency of choice. For this reason, as well as to enable you to change the economic reports on-the-fly from one monetary unit to another, SuperPro Designer offers to the user a databank of currencies where users need to keep the exchange rates between a foreign currency to US$. The exchange rate to US$ of a foreign currency (e.g. a Euro) represents how many monetary units of that foreign currency (Euros) can be fetched for one US$. You can add as many entries as you wish in your currencies databank, but you must specify only one as the 'default' currency of the databank. The choice for a default currency is going to be used as the automatic (default) choice for all prices stored in your 'User' database for any other resources (e.g. equipment purchase costs, per-hour labor costs, etc.) The default currency can be changed at any time. When you do change it, the application will offer you the choice to convert all prices currently stored in the 'User' database to the new 'default' currency of choice.


SuperPro Designer
The default currency in the DB has changed.
Would you like to convert the monetary values for all database entities to the new default currency?
Yes
No

If you answer 'Yes' then all monetary values (prices & cost items) in the 'User' database will be converted to the new default currency using the current values of exchange rates of the two currencies involved: the old default choice and the new choice.

15.12a Viewing the Contents of the Currencies Databank

To access the currencies databank, select the **Databanks ▸ Currencies** menu item from the main menu. The Currencies Databank Dialog that comes up, presents a table with all entries currently in the databank. Notice that you do not have to choose a database source (as required in most other databanks) as all records for currency exchange rates are only kept in the 'User' database.

15.12b Adding and Deleting Currencies

If you wish to add a new currency, simply click on the button and provide the name for the new currency (must be unique). After the new currency name is accepted, a new line will be entered with defaults for the new currency's symbol (the first five characters of the name) and exchange rate (1.0). You can simply click at the corresponding cells and edit the symbol and exchange rate to their proper values. Every currency you introduce in this databank, will be available as a choice in any process file (see 9.8 Currency) as part of the Currency Selection Dialog. If you wish to no longer keep a record on a specific currency, then select the line representing the currency you wish to delete and click on the button.

15.13 SITES & RESOURCES DATABANK

Eventually, every process (or recipe) is going to be carried out in a facility somewhere. The facility may be part of your own organization or it may be used on a contract basis from another corporation. SuperPro Designer allows you to describe such facilities and the resources available to them (e.g., equipment, usage fees, utilities, etc.) and keep their description in the 'User' database. Once a site and its resources exist in the 'User' database, a SuperPro Designer user can opt to take advantage of the allocation feature (see 6.1i Equipment Allocation and 'Section Allocation' on page 8-6) to map resources utilized in a process simulation project directly onto database entities that represent the resources as they exist in the actual manufacturing environment. The benefit of allocating a process and its resources to actual database sites and resources is that every user of the organization using SuperPro Designer will be forced to use the available resources consistently without making unrealistic assumptions and without using incorrect economic parameters. The 'User' database that comes with the software, contains only a couple of sample site descriptions, just so support one of the examples provided with the software that demonstrate the allocation feature (part of the 'SynPharm' group of process files). It is up to the users to populate their 'User' databases with database sites and resources that reflect the facilities where their SuperPro Designer simulated processes will be carried out.

15.13a Database Site (aka Database Facility)

A database site or sometimes referred to as a database facility is an entity created in the 'User' database that represents a processing (manufacturing) site. It can be as small as a room in a building or as large as a multi-acre industrial plant. In any case, a database site represents the

manufacturing environment that a recipe (or parts of it) may be carried out. For some large recipes, portions of them may be carried out in a given facility. Then, the intermediate product(s) may be stored and/or shipped to another facility (locally or remotely) where the rest of the recipe may be carried out in. For this reason, a SuperPro Designer recipe may be broken down into sections (see 8.1 Sections & Branches) and each section can be allocated to a database site of its own.

Every database site kept in the 'User' database, retains the following information:

- A parent site: typically that is a site that 'owns' the current site (or, in other words, a site that contains the current site).
- Capital Investment - related parameters (factors): piping, insulation, engineering, etc.
- Operating Cost - related parameters (factors): facility rental rates, insurance & local tax factors, etc.
- A set of description fields (location, contact person, comments, etc.)
- A number of contained resources (equipment, labor, heat transfer agents, power); for each resource added to the site, besides its operational characteristics (size for equipment, supply/return temperatures for heat transfer agents, etc.) users can also maintain availability limits (constraints) for rates and/or cumulative amounts (if applicable).

Database site descriptions are kept in the 'User' database in a hierarchical, tree-like organization (see Figure 15.1). In that way, every site created has been assigned to a 'parent site' and may have one or more 'contained sites'. This hierarchical organization allows a user to express the fact that a large manufacturing site (e.g., 'Site-A' in Figure 15.1), can be made up of several buildings or areas (I, II, III, IV,...). Each building could be made up of several floors (I-A, I-B, I-C,…, II-A, II-B, II-C,..., etc.)

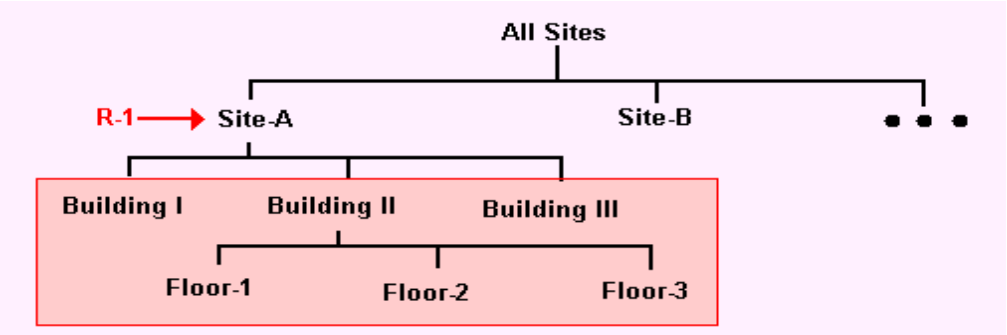


Figure 15.1: Hierarchical organization of database sites.

By organizing database sites in a hierarchy like shown above, users can take advantage of the two inheritance principles applied by SuperPro Designer to the sites databank:

1. Every resource defined at a given level in the site hierarchy is also available to any of its sub-sites (at all levels). For example, in Figure 15.1 shown above, having 'R-1' as an equipment resource defined at the 'Site-A' level, makes it automatically available to 'Building I', to 'Building-II' and 'Building III' as well as in 'Floor-1', 'Floor-2', 'Floor-3'.

2. Every sub-site automatically inherits all economic properties (cost factors) of its parent facility. However, if so desired, the factors can be overwritten locally too (see Site Properties Dialog: Capital Investment Tab and Site Properties Dialog: Operating Cost Tab).

Besides keeping the definition of resources, a site can also be the entity that maintains several economic factors that directly affect either the DFC estimation for a new site mimicking the one that is described in the database (see Capital Investment Dialog: DFC Tab), or the facility-dependent component of a recipe's operating cost (see 9.3f Facility-Dependent Cost) set to be executed using the existing database site. Very often, the facility-dependent component is not gathered by adding up the depreciation and maintenance cost of each equipment, but instead it is computed on a more lumped basis using a 'usage factor' for either the equipment involved or perhaps the site that is involved to carry out the recipe (see Operating Cost Adjustments Dialog: Facility Tab). Such 'usage' or 'rental' factors can be stored in the database, thereby securing that if different users within the organization assume the use of the same facility, they all use the same 'usage rates'. Other economic factors (costs) that can be saved as part of a database site description may be: the cost of resources (such as labor, utilities, etc.), estimation of maintenance, etc. All such factors are directly involved in the economic evaluation of a process and when stored directly in the 'User' database, make it easier for multiple users make consistent use in their own project evaluations.

A database facility may represent a real manufacturing facility or a hypothetical (or typical) manufacturing facility at a given location. In an era where global manufacturing is becoming more and more common, it may be beneficial to store a collection of database sites. Each site may represent a 'typical manufacturing facility' in a given locale, and therefore each site may capture different economic data (as they pertain to each locale). Once all these economic figures are readily accessible by all users of the program within an organization, it becomes an easy exercise to evaluate how the economics of a process change if the allocated site for the recipe (or parts there of) change from one site to another.

After a new section allocation (or re-allocation) assignment is made make sure you visit the Economic Data After Allocation Change Dialog to specify which (if any) of the database site object's economic properties you wish to copy over to the process section's properties.

15.13b Viewing the Contents of the Sites Databank

To see the list of currently defined database sites (facilities), select **Databanks ▸ Sites and Resources** from the main menu (or hit **F8** as a shortcut). From the Sites & Resources Databank Dialog that appears, you can view (and edit) the properties of existing sites by selecting the node representing the site in the left pane and then clicking on the button (above the same pane). Alternatively, you can right-click over the site's node and select **Edit Site Data** from the ensuing menu or just double-click on the node as a shortcut. The properties of the database site represented by that node appear in the Site Properties Dialog. You can also add or delete a site (see 15.13c Adding or Deleting a Site) or add resources to an existing database site (see 15.13d Adding, Deleting or Editing Database Resources).

15.13c Adding or Deleting a Site

From the Sites & Resources Databank Dialog, first select the database site that will be the parent of (or will 'own') the soon-to-be-created site and then click on the button as displayed over the left pane. Or, right-click over the parent of the soon-to-be-created site and

from the ensuing menu select **Add New Site** (when the parent node is 'All Sites') or **Add Sub-Site** (when the parent node is any other site).The Site Properties Dialog will appear. After you describe the new site's properties, click on **OK**. Notice that a new node will be added to the parent site's hierarchy displayed in the left pane of the dialog. If you wish to delete a database site, first select the node representing the site and then click on the ✕ button (as shown over the left pane of the dialog).

15.13d Adding, Deleting or Editing Database Resources

Database resources must be added to an existing database site (facility). First select the node that represents the facility in the left pane of the Sites & Resources Databank Dialog. This action will display in the right pane, all resources currently defined for that site. The resources are organized around the following four categories (folders):

1. Equipment
2. Heat Transfer Agents
3. Labor
4. Power

To add a resource, first select the category (one the four mentioned above) and then click on the button as displayed over the right pane of the dialog (or right-click over the folder icon and select **Add Equipment** or **Add Labor** etc. from the ensuing menu). Depending on the resource category you selected, one of the following dialogs will appear:

- New Site-Equipment Dialog (when introducing a new equipment)
- Add Heat Transfer Agent Dialog (when introducing a new heat transfer agent resource)
- Add Labor Type Dialog (when introducing a new labor resource)
- Add Power Type Dialog (when introducing a new power resource)

After exiting the new resource definition dialog with **OK**, notice that a new node will be added under the corresponding folder.

After you have introduced a labor type in a site (e.g. 'QC Operator'), you can also introduce 'staff' to represent specific individuals (e.g. "John Q.", "Jane M.", etc.) who belong in a given labor type perhaps with special skills that you may choose to engage in specific labor assignments (instead of simply choosing 'QC Operator'). To introduce a staff member, select the labor type node (under the site's name on the right-hand site tree), and select ***Add Staff*** *from its command menu (or click on the button displayed above the tree). Fill in the Labor Type Properties Dialog that will be presented and exit with* **OK**. *A new node will be added (under the labor type node) to represent the newly created staff member. This staff member will be available as an option to all labor engagements for operations in procedures that belong to a process section allocated to this site (see also 'Section Allocation' on page 8-6.)*

You can always view and/or edit the properties of any of the database resource entities by selecting the node representing them and then clicking on the button (above the same pane). Alternatively, you can right-click over the resource's node and select **Edit Equipment Data** or **Edit Heat Transfer Agent Data** etc. from the ensuing menu or just double-click on

the node as a shortcut. You may also delete a resource by selecting it and then clicking on the ✕ button (above the same pane).

Deleting a database resource entity or even an entire database site does not affect any existing process files that may have utilized this database entity as a resource illation or section allocation target. All previous projects utilizing this database entity already contain a complete definition of every database site (or database resource) engaged in that simulation inside their document (file) and do not depend on the continued presence of such entities in the 'User' databank in order to continue to produce simulation results.

As is the case with all other database entities, when users make changes to the database site objects and/or their contained resources, their changes are never automatically propagated to any project files that may have used them as allocation targets. Since database sites and their contained resources may have been changed since the last time that were used by a project, when you open your project file, the descriptions of database entities contained in the file (if any sections and/or resources are allocated to database counterparts) may not match their current values. SuperPro Designer offers users a direct menu choice that will check for the consistency of any database site object descriptions (or database resource descriptions) contained in the file with their database counterparts (as they exist currently). To trigger this comparison, select **File ▸ Check Consistency with Site DB** from the main menu of the application. This will produce the Reconcile with Site DB Dialog where you can view any discrepancies and you will have options on how to reconcile any differences.

15.14 EQUIPMENT DATABANKS

Equipment descriptions are kept in the database as two distinct entity collections (databanks):

(a) Site-Equipment: These are equipment resources added to database sites. They are meant to represent actual units present in a facility that is represented already by a database site.

(b) Vendor-Equipment: They are meant to represent equipment spec sheets as offered by vendors (or manufacturers) but not currently owned by any database facility.

15.14a Site-Equipment Databank

Equipment descriptions (just like any resource) can be added to database sites from the Sites & Resources Databank Dialog. However, for equipment, since they are the most commonly allocated resources in a SuperPro Designer simulation, there is an alternative interface: the Site-Equipment Databank Dialog that appears when selecting **Databanks ▸ Equipment ▸ in Sites** from the main menu of the application (or hit **F4** as a shortcut). This interface offers many more specialized features over the common interface. You can customize the equipment type that you are interested in and you can hone in the database site that you wish to view its equipment and list them by type.

The site-equipment presented in the table of contents of the Site-Equipment databank will include not only the site-equipment (of the chosen type) defined in the selected site, but also in all of its sub-sites.

You may either pick a specific site, or select 'All Sites' to inspect the site-equipment contents of all sites in the database. Also, you may choose to view only equipment of certain type, or 'All Types'. If you select a line in the table of contents representing a site-equipment and then click on the **View/Edit Properties** ( ) button, you will be presented with the Site-Equipment Databank Dialog that can be used to view and/or edit the properties of the selected site-equipment. Also, if you click on the **Create/Add New** ( ) button you will be presented with the New Site-Equipment Dialog that allows you to introduce a new site-equipment. Finally, you can delete a site-equipment by selecting its line in the table of contents and click on the **Delete** ( ) button. Any changes you have made (adding or deleting site-equipment or editing values of existing equipment) are kept as part of the editing session of the dialog but are not made permanent (i.e. written in the 'User' database) until you:

(a) Exit the Site-Equipment databank dialog with **OK**, or

(b) Click on the **Save Records to Disk (**)button: this will deposit all changes made so far into the 'User' database but will not exit this session of the dialog (i.e. will keep the dialog open).

15.14b Vendor-Equipment Databank

SuperPro Designer allows you to store in the database equipment descriptions (spec sheets) as offered by equipment vendors or manufacturers. Unlike site-equipment, the databank of vendor-equipment is spread between the 'Designer' and the 'User' database. In other words, some equipment specs come pre-loaded in our 'Designer' database (and as such, they cannot be edited or deleted by the user). However, the 'Designer' database includes only a very small fraction of all the possible actual manufacturing equipment that can be bought in the open market. It is mainly there to serve as a demonstration of the use of this feature. Users are encouraged to populate their own 'User' database with such descriptions of equipment, especially for equipment types that are typically included in their own simulations and involve manufacturers (or vendors) preferred by their corporation.

To access the vendor equipment databank select **Databanks ▸ Equipment ▸ from Vendors** from the main menu (or hit **Shift+F4** as a shortcut). From the Vendor-Equipment Databank Dialog that appears you can view the contents of the vendor-equipment databank and add or delete new items. If you select a vendor-equipment coming from the 'Designer' database then you can only view (but not modify) the property values of that vendor equipment. First select in the table of contents the line that represents the vendor-equipment whose description you wish to view and then click on the **View Properties** ( ) button. You will be presented with the Vendor Equipment Properties Dialog in view-only mode: you can view the selected vendor-equipment's properties but you cannot change them. If you select a vendor-equipment from the 'User' database, then you will be able to view as well as modify the values of vendor equipment as they have been created previously by the user and kept in that databank. Select a vendor-equipment in the table of contents and click on the **View/Edit Properties** ( ) button and you will be presented with the Vendor Equipment Properties Dialog only this time you can view as well as modify (and save) the selected vendor-equipment's property values. You can also add new vendor equipment (click on the **Create/Add New** ( ) button and complete the New Vendor Equipment Dialog) as well as delete any existing definitions for

vendor-equipment that you no longer need (select the equipment line and click on the **Delete** (✕) button).

A new vendor-equipment introduced in the vendor-equipment databank can be associated with a specific vendor (or manufacturer). If a record of the proper manufacturer is not yet part of the databank of vendors and manufacturers please add it in first (see 15.14c Databanks of Equipment Vendors/Manufacturers). Also, the vendor-equipment description must include information on size and cost, but may also include a list of extra specifications that may be needed in order for the user to decide which type to use for a given application. The set of user-specifications can be extended to include practically any feature (see 15.14e Specification Variables Databank).

Any changes you have made (adding or deleting vendor equipment or editing values of existing vendor-equipment) are kept as part of the editing session of the dialog but are not made permanent (i.e. written in the 'User' database) until you:

(a) Exit the Vendor-Equipment databank dialog with **OK**, or

(b) Click on the **Save Records to Disk** ( )button: this will deposit all changes made so far into the 'User' database but will not exit this session of the dialog (i.e. will keep the dialog open).

15.14c Databanks of Equipment Vendors/Manufacturers

SuperPro Designer allows you to create a catalog of preferred equipment vendors and/or manufacturers that your corporation most commonly uses to purchase equipment for manufacturing. A sample of manufacturers comes pre-loaded in the 'Designer' database and as such, they cannot be edited or deleted by the user. However, the 'Designer' database includes only a very small fraction of all the possible equipment vendors and manufacturers that exist in the market. It is mainly there to serve as a demonstration of the use of this feature. Users are encouraged to populate their own 'User' database with such descriptions of vendors, especially those preferred by their own organization.

To access the databanks of vendors and manufacturers select **Databanks ▸ Equipment ▸ Vendors/Manufacturers** from the main menu (or hit **F5** as a shortcut). From the Equipment Vendor/Manufacturer Databank Dialog that appears you can view the contents of the equipment vendor/manufacturer databanks, and have a chance to edit, add or delete entries. Using the 'Database Filter..' button you may choose to display only the 'Designer' or the 'User' database vendors/manufacturers. If you select a vendor/manufacturer that resides in the 'Designer' database then you can only view (but not modify) the property values of that vendor/manufacturer (Click on the view button you will be presented with the Equipment Vendor/Manufacturer Data Dialog in view-only mode). If you choose a vendor/manufacturer that exists in the 'User' database, then you will be able to view as well as modify the values of vendor records as they have been created previously by the user and kept in that databank (click on you will be presented with the Equipment Vendor/Manufacturer Data Dialog). You can also add new vendor/manufacturer record (click on the button and complete the Equipment Vendor/Manufacturer Data Dialog) as well as delete any existing definitions for vendors/manufacturers that you no longer need (select the vendor/manufacturer line in the table of contents, and click on the ✕ button).

15.14d Equipment Types & Specifications

SuperPro Designer supports the use of many equipment types as hosts of procedures in process simulations. When describing an actual equipment to be included in the databank of site-equipment or an equipment specification sheet to be included in the vendor-equipment databank, the user is expected to provide a list of specifications that are necessary for the characterization of the equipment in a process simulation in a way that matches exactly the properties of that equipment when its sizing is set to 'Rating Mode' (see 6.1a Equipment Sizing (Design vs Rating Mode)). This set of specifications is called the '**Required Specs**'. However, if needed, users may also extend the definition of an equipment type by appending several more specifications that may be deemed necessary to retain for their records. This extra set of specifications (called '**User Specs**') can include any properties currently already in use (such as 'Diameter', 'Height', 'Filter Area' etc.) or users may introduce their own (see 15.14e Specification Variables Databank).

To view and/or edit the list of specifications for all equipment types supported by the application, use the **Databanks ▸ Equipment ▸ Types & Specifications** menu item from the main menu (or hit **F6** as a shortcut). You will be presented with the Equipment Types & Specifications Dialog where you may view the required specifications ('Required Specs') for a given equipment type (as expected by the application) as well as any 'User Specs' that may have been added by the user to a selected equipment type. The left-hand-side pane displays all equipment types recognized by the application and organized hierarchically in groups (Filters, Vessels/Reactors etc). Once you select a specific type, the right-hand-side pane displays the Required Specs and the User Specs for the selected equipment type. The list of Required Specs for a given equipment type is not editable. You cannot delete and/or add any new members to it. You may view the properties of any of the required specs by selecting it and clicking on . This will present the Specification Properties Dialog (in view-only mode). You may add your own specification by selecting the 'User-Specs' folder and then clicking on the **Create/Add New** ( ) button or right-clicking on the 'User-Specs' folder and selecting **Add Specs** from the menu. The Add Specification Dialog will appear from where you can describe the properties of the new specification. After exiting the dialog with **OK** a new node will be added the 'User Specs' folder and from now on, this new specification will be presented every time a user adds a new site-equipment or vendor-equipment (of the chosen type) in the 'User' databank.

If you cannot find an existing appropriate specification that needs to be added to the description of an equipment type, you can add your own, thereby extending the list of available specification options for this or any other equipment (see 15.14e Specification Variables Databank).

If you no longer need to have an existing 'User-Spec' associated with an equipment type, select the node (under the 'User-Specs' folder in the right pane) and click on the button. Editing, adding or deleting a specification as part of an equipment type description, will result in propagating the change to all records of site-equipment or vendor-equipment of this type in the 'User' database. However, these changes will not affect the descriptions of site-equipment or vendor-equipment already allocated in existing simulation files. If users wish to re-align the definitions of site-equipment or vendor-equipment kept in their files, they will have to do it manually (see Equipment Data Dialog: Allocation Tab).

15.14e Specification Variables Databank

In SuperPro Designer, every equipment type is characterized by a set of specification variables. When keeping records of equipment in database sites or as vendor-equipment in the database, the user must provide at least the essential features required to describe a piece of equipment in rating mode (these specifications are called 'Required Specs'). Furthermore, users may extend the description of equipment records with extra specifications ('User Specs') that keep features of equipment that need to be viewed by users as they may influence their decisions as to which instance they should engage. To provide those additional 'User Specs' users may utilize all existing specification definitions (already used by the application for the description of the 'Required Specs') or they can introduce new specifications that will be kept as part of the 'User' databank of specifications.

To access the specifications databanks select **Databanks ▸ Equipment ▸ Specification Variables** from the main menu (or hit **Shift+F6** as a shortcut). From the Specification Variables Databank Dialog that appear you can view the list of variable specifications that are currently available, as well as add more. Using the 'Database Filter..' button you may choose to display only the 'Designer' or the 'User' database specification variables. If you select a specifiation variable from the 'Designer' databse then you can only view (but not modify) its properties in the databnk. You may view all the attributes of the selected specification by clicking on button (you will be presented with the Specification Properties Dialog in view-only mode). If you select a specification variable that resides in the 'User' database, then you will be able to view as well as modify the values of specifications as they have been created previously by the user and kept in that databank (click on you will be presented with the Specification Properties Dialog in editing mode). You can also add new specification variables (click on the button and complete the Add Specification Dialog) as well as delete any existing specifications that you no longer need (select the speciation line in the table of contents and click on the button). Note that for a user-defined specification variable that is already used by either a site-equipment or a vendor-equipment currently recorded in the database, you will not be able to change its type or delete it from the databank. You will have first to remove it from all the 'User Specs' list that is currently in use, and then return to this interface to delete or modify it.

15.14f User Defined Cost Models Databank

Another important databank available in SuperPro Designer is the User Defined Cost Models Databank. User defined cost models (UDCMs) are used to better estimate the cost of a piece of a equipment if the built-in model produces unacceptable results. For more information on how to request to have the purchase cost be calculated using your own UDCM, please see The User-Defined Cost Model (UDCM). These models with their properties will be kept in the 'User' database. UDCMs can be added to your databank two ways:

(a) First define a UDCM locally (with scope restricted to the process file alone) for an existing equipment and later export (deposit) it to the UDCM databank, or

(b) Introduce a UDCM for a given equipment type directly in the UDCM databank.

In both cases the cost models are ultimately saved in the 'User' database file and grouped by equipment type.

To view and edit the list of available user defined cost models select **Databanks ▸ Equipment ▸ Specification Variable** from the main menu of the program. You will be

presented with the Equipment User Defined Cost Models Databank Dialog, where you may see a list of all available cost models defined in the 'User' and 'Designer' databases for the currently selected equipment type. Using the 'Database Filter...' button you may choose to display the cost models of the 'Designer,' the 'User' or both databases. Select a user cost model from the list (table row is highlighted in black) and whether the model exists in the 'Designer' or the 'User' database click on the view button or the view/edit button respectively. The User-Defined Cost Model Dialog will apear where you may view and/or edit the property values of the selected cost model. Finally you may also delete the user defined cost models residing in the 'User' database by clicking on the delete button.

15.15 PROCESSES DATABANK

As you work with SuperPro Designer for a long time, you will accumulate several completed projects (files). Before you start a new project, you may benefit from reviewing a previously completed simulation as it may have some feature(s) common to a previously completed, tested and approved simulation. Therefore, you need to have the means to search across all of your completed project files in hopes of finding the one(s) that may be of interest. Since the '.spf' files used by SuperPro Designer to save the contents of a project are binary and therefore not amenable to a search by typical search tools, SuperPro Designer offers you a more efficient solution: the 'Process' database. The 'Process' database file is used to contain exclusively the processes databank. Each member of the processes databank is a complete description of a process simulation file but in a database (MS-Access) format. Essentially the processes databank can be viewed as a huge catalog where past simulation projects are archived in a way that makes them easy to search and locate a specific record that matches some search criteria. As part of the process record deposited in the processes databank, besides information about materials, unit operations, equipment, etc. that participate in the process, SuperPro Designer also allows you to associate several keywords that may help you locate this process in a later search. Even the location of the actual '.spf' file is kept as one of the process record fields stored in the databank. The 'Processes' databank may be of greater importance to corporate users, as it can be used as the means to make completed projects available to others in the corporation along with an interface that allows them locate a given record based on some concrete search criteria.

In order to be able to deposit a process description in the database, you must assume a user name. That name will be kept in association with the process record. You can inform the application what to use as a user name when accessing the 'Process' database (or any other database that requires it) by selecting **File ▸ Application Settings** from the main menu and visiting the Application Settings Dialog: Miscellaneous tab.

15.15a Adding a Process Record in the Processes Databank

After you have completed your simulation project with SuperPro Designer you may then deposit the completed process into the processes databank. Select **Databanks ▸ Processes ▸ Export Current Process** from the main menu. The will bring up the Export to the Process Databank Dialog. From this dialog you may set a name (must be unique as it will be used as an index in the database), a brief textual description of the process and several keywords that will help identify the process record later when you search from the Process DB: Search Dialog.

The ‘User Name’ field is required and it is kept associated with the process record as a reminder of the engineer that entered the record in the processes databank. If you haven’t selected a user name yet, you can do so from the Application Settings Dialog: Miscellaneous tab.

15.15b .Viewing the Process Records in the Processes Databank

To view all the contents of the processes databank, select **Databanks ▸ Processes ▸ View** from the main menu. You will be presented with the Process DB: View Contents Dialog where you can see a listing of all processes that have been registered (entered) in the processes databank. The process record is represented by its name that was used when the record was deposited in the databank. When you select a process record by clicking on a row in the table, the interface will display further information such as the user who created it, the creation and last modification dates, the main product name and main product rate or size (if defined) and additional info which may be relevant to the file.

15.15c Searching in the Processes Databank

When you need to search through the repository of all process records, select **Databanks ▸ Processes ▸ Search**. The Process DB: Search Dialog that will appear will allow you to provide search criteria to be used to conduct a search in the process database in order to find any records that match. The search criteria that can currently be used are:

- The ‘name’ of the process record.
- The ‘user name’ associated with the process record.
- The ‘main product name’
- The ‘keywords’ associated with the process record.
- The ‘main product rate’ (or size) be larger or smaller than a certain value.

All of the above criteria are logically ‘AND’ed together and the result of the search is displayed in the table shown at the bottom of the dialog.

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